



# Adiabatic approximation for a two-level atom in a light beam

Amandine Aftalion, Francis Nier

## ► To cite this version:

Amandine Aftalion, Francis Nier. Adiabatic approximation for a two-level atom in a light beam. 2011.  
hal-00641565v2

**HAL Id: hal-00641565**

**<https://hal.science/hal-00641565v2>**

Preprint submitted on 23 Jan 2012

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Adiabatic approximation for a two-level atom in a light beam

Amandine Aftalion\* and Francis Nier†

January 23, 2012

**Abstract:** Following the recent experimental realization of synthetic gauge potentials, Jean Dalibard addressed the question whether the adiabatic ansatz could be mathematically justified for a model of an atom in 2 internal states, shone by a quasi resonant laser beam. In this paper, we derive rigorously the asymptotic model guessed by the physicists, and show that this asymptotic analysis contains the information about the presence of vortices. Surprisingly, the main difficulties do not come from the nonlinear part but from the linear Hamiltonian. More precisely, the analysis of the nonlinear minimization problem and its asymptotic reduction to simpler ones, relies on an accurate partition of low and high frequencies (or momenta). This requires to reconsider carefully previous mathematical works about the adiabatic limit. Although the estimates are not sharp, this asymptotic analysis provides a good insight about the validity of the asymptotic picture, with respect to the size of the many parameters initially put in the complete model.

**Résumé :** Suite à la réalisation expérimentale de champs de jauge artificiels, Jean Dalibard a soulevé la question de l'approximation adiabatique pour un modèle d'atome à deux niveaux, éclairé par un faisceau laser résonnant. Dans cet article, nous dérivons rigoureusement le modèle asymptotique deviné par les physiciens et montrons que cette analyse contient l'information sur la présence de vortex. Les difficultés, et c'est une surprise, ne viennent pas du terme non linéaire. Plus précisément, l'analyse du problème non linéaire, et la réduction asymptotique à un modèle plus simple, reposent sur une séparation précise des grandes et basses fréquences (ou grands et bas moments). Cela nécessite de reconsidérer avec soin les résultats mathématiques existants sur la limite adiabatique. Bien que les estimations ne soient pas optimales, elles fournissent une bonne intuition sur la validité du modèle asymptotique, par rapport aux tailles des différents paramètres initialement mis dans le modèle.

---

\*CNRS & Université Versailles-Saint-Quentin-en-Yvelines, Laboratoire de Mathématiques de Versailles, CNRS UMR 8100, 45 avenue des États-Unis, 78035 Versailles Cedex, France

†1) IRMAR, Université de Rennes 1, 35042 Rennes Cedex, France. 2) CERMICS, INRIA project-team MICMAC.

# 1 Introduction

A lot of interest, both in the mathematical and physical community, has been devoted in the past 10 years to the study of the rotation of a Bose Einstein condensate: experiments [MCWD1, MCWD2], theoretical works (see [Coo, Fet] for reviews), mathematical contributions [Aft, LiSe]. In the first experimental production of such rotating Bose Einstein condensates, a rotating laser beam was superimposed on the magnetic trap holding the atoms in order to spin up the condensate by creating a harmonic anisotropic rotating potential [MCWD1, MCWD2]. Recently, a new experimental device has emerged which consists in realizing artificial or synthetic gauge magnetic forces and leads to the formation of vortex lattices at rest in the lab frame [LCGPS]. A colloquium [DGJO] has analyzed in detail the artificial gauge fields and their manifestations. In order to understand the main ingredients of the physics of geometrical gauge fields, [DGJO] (see also [GCYRD]) study the case of a single quantum particle state with a 2 levels internal structure. More complex systems with more than 2 internal levels are also discussed in [DGJO] but we stick here to the simpler case of 2 levels, which contains all the mathematical difficulties. A key issue is to determine whether one internal state can be followed adiabatically. A question raised by Jean Dalibard is to analyze in particular whether vortex formation may break down the adiabatic process. In [DGJO], some conditions are provided, that we want to analyze from a mathematical point of view.

We are interested in the minimization of the energy

$$\begin{aligned} \mathcal{E}_\kappa(\phi) = & \int_{\mathbb{R}^2} |\nabla \phi|^2 + V_\kappa(x, y) |\phi|^2 + \frac{G}{2} |\phi|^4 \, dx dy \\ & + \Omega_{\kappa, \ell_\kappa}(x) \langle \phi, \begin{pmatrix} \cos(\theta_{\ell_\kappa}(x)) & e^{i\varphi_\kappa(y)} \sin(\theta_{\ell_\kappa}(x)) \\ e^{-i\varphi_\kappa(y)} \sin(\theta_{\ell_\kappa}(x)) & -\cos(\theta_{\ell_\kappa}(x)) \end{pmatrix} \phi \rangle_{\mathbb{C}^2}, \end{aligned}$$

where  $\phi = \begin{pmatrix} \phi_1(x, y) \\ \phi_2(x, y) \end{pmatrix} \in \mathbb{C}^2$  and  $|\phi(x, y)|^2 = |\phi_1(x, y)|^2 + |\phi_2(x, y)|^2$ . We prescribe that the  $L^2$  norm of  $\phi$  is 1. Here  $\phi_1$  and  $\phi_2$  are the internal degree of freedom of a particle: ground and excited state of the atom. It is assumed that the atom is shone by a quasi resonant laser beam. The functions  $\Omega_{\kappa, \ell_\kappa}(x)$ ,  $\varphi_\kappa(y)$  and  $\theta_{\ell_\kappa}(x)$  are given as in [DGJO] by

$$\begin{aligned} \Omega_{\kappa, \ell_\kappa}(x) &= \kappa \Omega\left(\frac{x}{\ell_\kappa}\right) \text{ with } \Omega(x) = \sqrt{1+x^2}, \\ \theta_{\ell_\kappa}(x) &= \underline{\theta}\left(\frac{x}{\ell_\kappa}\right) \text{ with } \cos(\underline{\theta}(x)) = \frac{x}{\sqrt{x^2+1}} \quad , \quad \sin(\underline{\theta}(x)) = \frac{1}{\sqrt{x^2+1}}, \\ \varphi_\kappa(y) &= \underline{\varphi}(ky) \text{ with } \underline{\varphi}(y) = y, \end{aligned}$$

where  $\underline{\varphi}$  is the phase of the propagating laser beam while  $\underline{\theta}$  is the mixing angle. We define

$$M(x, y) = \Omega(x) \begin{pmatrix} \cos(\underline{\theta}(x)) & e^{i\underline{\varphi}(y)} \sin(\underline{\theta}(x)) \\ e^{-i\underline{\varphi}(y)} \sin(\underline{\theta}(x)) & -\cos(\underline{\theta}(x)) \end{pmatrix}. \quad (1.1)$$

The matrix  $M$  models the coupling between the atom and the laser. The  $2 \times 2$  matrix  $M(\frac{x}{\sqrt{\ell_\kappa k}}, \sqrt{\ell_\kappa k} y)$  can be diagonalized in the bases  $(\psi_+, \psi_-)$  respectively associated with the eigenvalues  $\pm \Omega(x)$ ,

$$\psi_+ = \begin{pmatrix} C \\ S e^{-i\varphi} \end{pmatrix}, \quad \psi_- = \begin{pmatrix} S e^{i\varphi} \\ -C \end{pmatrix}, \quad (1.2)$$

with  $C = \cos\left(\frac{1}{2}\theta\left(\frac{x}{\sqrt{\ell_\kappa k}}\right)\right)$ ,  $S = \sin\left(\frac{1}{2}\theta\left(\frac{x}{\sqrt{\ell_\kappa k}}\right)\right)$  and  $\varphi = \sqrt{\ell_\kappa k} y$ . When the particle follows adiabatically the eigenstate  $\psi_-$ , this corresponds to set formally  $\phi = u(x, y)\psi_-$ , where  $u(x, y) \in \mathbb{C}$  in  $\mathcal{E}_\kappa$ . Then  $u$  minimizes a Gross-Pitaevskii type energy functional with a modified trapping potential called the geometrical gauge potential. The scalar potential  $V_\kappa(x, y) = V_\kappa(x, y) \text{Id}_{\mathbb{C}^2}$  will be adjusted in order to produce a harmonic potential after the addition of the geometrical gauge potential from the adiabatic theory. We want to justify the adiabatic approximation for states close to  $\psi_-$  and analyze the error term between the initial and effective Hamiltonians.

After a rescaling, the parameter occurring in the experiments have the following orders of magnitude

$$\kappa \sim 10^6, \quad G \sim 600, \quad \ell_\kappa \sim 25, \quad k \sim 50,$$

but other values can be discussed. Conditions on the strength and spatial extent of the artificial potential have to be prescribed in order to induce large circulation. Two cases,  $\ell_\kappa k \geq 1$  and  $\ell_\kappa k \leq 1$ , can be distinguished and the problem has to be rewritten in two different ways in order to apply semiclassical techniques. In fact, we will focus on the case  $\ell_\kappa k \geq 1$ , corresponding to the previous numerical values. The complete analysis is carried out in the asymptotic regime  $\ell_\kappa k \rightarrow +\infty$  but some partial results are also valid for  $\ell_\kappa k \leq 1$  or  $\ell_\kappa k \rightarrow 0$ .

A change of scale  $\phi(x, y) = \sqrt{\frac{k}{\ell_\kappa}} \psi\left(\sqrt{\frac{k}{\ell_\kappa}} x, \sqrt{\frac{k}{\ell_\kappa}} y\right)$  yields a new expression for the energy:

$$\begin{aligned} & \int_{\mathbb{R}^2} \frac{k}{\ell_\kappa} (|\partial_x \psi|^2 + |\partial_y \psi|^2) + V_\kappa\left(\sqrt{\frac{\ell_\kappa}{k}} x, \sqrt{\frac{\ell_\kappa}{k}} y\right) |\psi|^2 \\ & + \kappa \Omega\left(\frac{x}{\sqrt{k\ell_\kappa}}\right) \langle \psi, \begin{pmatrix} \cos\left(\theta\left(\frac{x}{\sqrt{k\ell_\kappa}}\right)\right) & e^{i\varphi(\sqrt{k\ell_\kappa} y)} \sin\left(\theta\left(\frac{x}{\sqrt{k\ell_\kappa}}\right)\right) \\ e^{-i\varphi(\sqrt{k\ell_\kappa} y)} \sin\left(\theta\left(\frac{x}{\sqrt{k\ell_\kappa}}\right)\right) & -\cos\left(\theta\left(\frac{x}{\sqrt{k\ell_\kappa}}\right)\right) \end{pmatrix} \psi \rangle_{\mathbb{C}^2} \\ & + \frac{Gk}{2\ell_\kappa} |\psi|^4 \, dx dy. \end{aligned}$$

According to the two cases  $\ell_\kappa k \geq 1$  or  $\ell_\kappa k \leq 1$ , we define a small parameter  $\varepsilon$  that allows to rescale the energy. In fact, we define rather the parameter  $\varepsilon^{2+2\delta}$ , where  $\delta$  can be taken as a first step equal to  $5/2$ . The exponent  $\delta > 0$  is a technical trick which provides the right quantitative estimates for the adiabatic approximation with a quadratic kinetic energy term. The suitable choice of this new parameter  $\delta$  is discussed further down in this introduction, in Subsections 1.1 and 1.2. The small parameter  $\varepsilon > 0$  is thus introduced according to the two cases:

if  $\ell_\kappa k \geq 1$ , then

$$\varepsilon^{2+2\delta} = \frac{k^2}{\kappa}, \quad \delta > 0, \quad G_\varepsilon = \frac{Gk}{\kappa\ell_\kappa} = \frac{G}{k\ell_\kappa} \varepsilon^{2+2\delta}; \quad (1.3)$$

(This leads in our example to  $\varepsilon^{2+2\delta} = 2.5 \cdot 10^{-3}$ .)

if  $\ell_\kappa k \leq 1$ , then

$$\varepsilon^{2+2\delta} = \frac{1}{\ell_\kappa^2 \kappa}, \quad \delta > 0, \quad G_\varepsilon = \frac{Gk}{\kappa\ell_\kappa} = Gk\ell_\kappa \varepsilon^{2+2\delta}. \quad (1.4)$$

We define

$$\tau = (\tau_x, \tau_y) = \begin{cases} (\frac{1}{k\ell_\kappa}, 1) & \text{if } k\ell_\kappa \geq 1, \\ (1, k\ell_\kappa) & \text{if } k\ell_\kappa \leq 1. \end{cases} \quad (1.5)$$

In both cases, this leads to

$$\kappa^{-1} \mathcal{E}_\kappa(\phi) = \mathcal{E}_\varepsilon(\psi) \quad (1.6)$$

where

$$\mathcal{E}_\varepsilon(\psi) = \langle \psi, H_{Lin} \psi \rangle + \frac{G_{\varepsilon,\tau}}{2} \int |\psi|^4 dx dy, \quad (1.7)$$

$$G_{\varepsilon,\tau} = G\tau_x \tau_y \varepsilon^{2+2\delta}, \quad (1.8)$$

and

$$H_{Lin} = -\varepsilon^{2\delta} \tau_x \tau_y \varepsilon^2 \Delta + V_{\varepsilon,\tau}(x, y) + M(\sqrt{\frac{\tau_x}{\tau_y}} x, \sqrt{\frac{\tau_y}{\tau_x}} y), \quad (1.9)$$

$$V_{\varepsilon,\tau}(x, y) = \kappa^{-1} V_\kappa(\sqrt{\frac{\ell_\kappa}{k}} x, \sqrt{\frac{\ell_\kappa}{k}} y) \quad (\text{to be fixed}). \quad (1.10)$$

The quadratic energy (linear Hamiltonian) is

$$\begin{aligned} \mathcal{E}_{quad,\varepsilon}(\psi) &= \int_{\mathbb{R}^2} \varepsilon^{2+2\delta} \tau_x \tau_y |\nabla \psi|^2 + V_{\varepsilon,\tau}(x, y) |\psi|^2 \\ &\quad + \langle \psi, M(\sqrt{\frac{\tau_x}{\tau_y}} x, \sqrt{\frac{\tau_y}{\tau_x}} y) \psi \rangle_{\mathbb{C}^2} dx dy \end{aligned} \quad (1.11)$$

$$= \langle \psi, H_{Lin} \psi \rangle. \quad (1.12)$$

At least when  $\tau_x = \tau_y = 1$  and  $\delta = 0$ , this problem looks like the standard problem of spatial adiabatic approximation studied in [Sor], [MaSo], [MaSo2] [PST], although it requires some adaptations because the symbols are neither bounded nor elliptic.

We shall consider the asymptotic analysis as  $\varepsilon \rightarrow 0$  with uniform control with respect to the parameters  $G, k\ell_\kappa$  which allow to fix the range of validity of the reduced models. Then we shall consider the asymptotic behaviour of the reduced model and the whole system as  $\ell_\kappa k$  is large. Specifying the right assumptions on  $V_{\varepsilon,\tau}(x, y)$  or  $V_\kappa$ , possibly in a scale depending on  $(\ell_\kappa, k)$ , is also an issue.

## 1.1 Main result for the Gross-Pitaevskii energy

We shall choose the potential  $V_{\varepsilon, \tau}$  in (1.10) such that after the addition of the adiabatic potential in the lower energy band, the effective potential is almost harmonic. Namely, we assume

$$V_{\varepsilon, \tau}(x, y) = \frac{\varepsilon^{2+2\delta}}{\ell_V^2} v(\sqrt{\tau_x}x, \sqrt{\tau_y}y) + \sqrt{1 + \tau_x x^2} - \varepsilon^{2+2\delta} \left[ \frac{\tau_x^2}{(1 + \tau_x x^2)^2} + \frac{1}{1 + \tau_x x^2} \right], \quad (1.13)$$

with the potential  $v$  chosen such that

$$\begin{aligned} v(x, y) &= (x^2 + y^2)\chi_v(x^2 + y^2) + (1 - \chi_v(x^2 + y^2)) \\ \chi_v &\in \mathcal{C}_0^\infty([0, 2)) \quad , \quad 0 \leq \chi_v \leq 1, \quad \chi_v \equiv 1 \text{ on } [0, 1], \end{aligned} \quad (1.14)$$

and  $\ell_V > 0$  parametrizes the shape of the quadratic potential around the origin. With these assumptions on the potential  $V_{\varepsilon, \tau}$ , if one chooses  $\psi = u(x, y)\psi_-$ , where  $\psi_-$  is the eigenfunction corresponding to  $-\Omega(x\sqrt{\tau_x/\tau_y})$  of the matrix  $\Omega(x\sqrt{\tau_x/\tau_y})M(x\sqrt{\tau_x/\tau_y}, y\sqrt{\tau_y/\tau_x})$ , then the linear part  $H_{Lin}$  in  $\mathcal{E}_\varepsilon$  is formally replaced by the scalar  $\varepsilon^{2+2\delta}\tau_x\hat{H}_-$  where

$$\hat{H}_- = -\partial_x^2 - \left( \partial_y - i \frac{x}{2\sqrt{1 + \tau_x x^2}} \right)^2 + \frac{1}{\ell_V^2 \tau_x} v(\sqrt{\tau_x}x, \sqrt{\tau_y}y). \quad (1.15)$$

In the limit  $\tau_x \rightarrow 0$ , a natural  $(\varepsilon, \tau)$ -independent scalar reduced model emerges:

$$\mathcal{E}_H(u) = \langle u, \left[ -\partial_x^2 - \left( \partial_y - \frac{ix}{2} \right)^2 + \frac{x^2 + y^2}{\ell_V^2} \right] u \rangle + \frac{G}{2} \int_{\mathbb{R}^2} |u|^4, \quad u(x, y) \in \mathbb{C}.$$

Because  $\kappa$  is large, or  $\varepsilon$  is small, it is natural to expect that the ground state of  $\mathcal{E}_\varepsilon$  is close, up to a unitary transform, to a vector  $u(x, y)\psi_-$ . This is the aim of the adiabatic theory and leads to a scalar problem. In order to get good bounds on the energy, we need to study the limit  $\tau_x$  small at the same time.

In all our work  $\ell_V > 0$  and  $G > 0$  are assumed to be fixed, while the asymptotic behaviour is studied as  $\varepsilon \rightarrow 0$  and  $\tau_x \rightarrow 0$ .

The quadratic part of the above energy is associated with the Hamiltonian

$$H_{\ell_V} = -\partial_x^2 - \left( \partial_y - \frac{ix}{2} \right)^2 + \frac{x^2 + y^2}{\ell_V^2}, \quad (0 < \ell_V < +\infty), \quad (1.16)$$

with the domain

$$\mathcal{H}_2 = \left\{ u \in L^2(\mathbb{R}^2), \quad \sum_{|\alpha|+|\beta|\leq 2} \|q^\alpha D_q^\beta u\|_{L^2} < +\infty \right\}, \quad q = (x, y) \in \mathbb{R}^2, \quad (1.17)$$

endowed with the norm  $\|f\|_{\mathcal{H}_2}^2 = \sum_{|\alpha|+|\beta|\leq 2} \|q^\alpha D_q^\beta u\|_{L^2}^2$  and the corresponding distance  $d_{\mathcal{H}_2}$ . It is not difficult (see Section 4.2) to check that the minimization of  $\mathcal{E}_H(\varphi)$  under the constraint  $\|\varphi\|_{L^2} = 1$ , admits solutions and that the set,  $\text{Argmin } \mathcal{E}_H$ , of ground states for  $\mathcal{E}_H$  is a bounded set of  $\mathcal{H}_2$ .

**Definition 1.1.** For a functional  $\mathcal{E}$  defined on a Hilbert space  $\mathcal{H}$  (with  $+\infty$  as a possible value), we set

$$\mathcal{E}_{\min} = \inf_{\|u\|_{L^2}=1} \mathcal{E}(u) \quad \text{and} \quad \text{Argmin } \mathcal{E} = \{u \in \mathcal{H}, \mathcal{E}(u) = \mathcal{E}_{\min} \text{ and } \|u\|_{L^2} = 1\}.$$

**Theorem 1.2.** Fix the constant  $\ell_V, G$  and  $\delta$  and assume, for some  $C_\delta = C(\ell_V, G, \delta) > 0$ ,

$$\varepsilon^{2\delta} \leq \frac{\tau_x^{\frac{5}{3}}}{C_\delta}. \quad (1.18)$$

Let  $\chi = (\chi_1, \chi_2)$  be a pair of cut-off functions such that  $\chi_1^2 + \chi_2^2 \equiv 1$  on  $\mathbb{R}^2$ ,  $\chi_1 \in C_0^\infty(\mathbb{R}^2)$  and  $\chi_1 = 1$  in a neighborhood of 0.

There exists  $\nu_0 = \nu_{\ell_V, G} \in (0, \frac{1}{2}]$  and for any given  $\delta > 0$ , there are constants  $\tau_\delta = \tau(\ell_V, G, \delta) > 0$ ,  $C_{\chi, \delta} = C(\ell_V, G, \delta, \chi) > 0$ , and a unitary operator  $\hat{U} = \hat{U}(\varepsilon, \tau, \ell_V, G, \delta)$  which guarantee the following properties

- The energy  $\mathcal{E}_\varepsilon$  introduced in (1.7) admits ground states as soon as  $\tau_x \leq \tau_\delta$ , with

$$|\mathcal{E}_{\varepsilon, \min} - \varepsilon^{2+2\delta} \tau_x \mathcal{E}_{H, \min}| \leq C_\delta \varepsilon^{2+2\delta} \tau_x^{\frac{5}{3}}.$$

- For any  $\psi \in \text{Argmin } \mathcal{E}_\varepsilon$  written in the form  $\psi = \hat{U} \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$ , the vector  $a = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}$  satisfies

$$\|a_+\|_{L^2} \leq C_\delta \varepsilon^{2+2\delta} \tau_x, \quad \|a\|_{H^2} \leq \frac{C_\delta}{\tau_x}, \quad \|a\|_{L^4} + \|a\|_{L^6} \leq C_\delta,$$

$$\|\chi_2(\tau_x^{\frac{1}{9}} \cdot) a_-\|_{L^2} \leq C_{\chi, \delta} \tau_x^{\frac{1}{3}},$$

$$d_{\mathcal{H}_2}(\chi_1(\tau_x^{\frac{1}{9}} \cdot) a_-, \text{Argmin } \mathcal{E}_H) \leq C_{\chi, \delta} (\tau_x^{\frac{2\nu_0}{3}} + \varepsilon),$$

$$\|a_+\|_{L^\infty} \leq C_\delta \varepsilon^{1+\delta}, \quad d_{L^\infty}(\chi_1(\tau_x^{\frac{1}{9}} \cdot) a_-, \text{Argmin } \mathcal{E}_H) \leq C_{\chi, \delta} (\tau_x^{\frac{2\nu_0}{3}} + \varepsilon)^{\frac{1}{2}}.$$

All the constants can be chosen uniformly with respect to  $\delta \in (0, \delta_0]$  for any fixed  $\delta_0 > 0$ .

**Remark 1.3.** The proof is made in two steps: 1) the limit  $\varepsilon \rightarrow 0$  corresponds to the adiabatic limit for the linear problem and allows to replace the linear part  $H_{Lin}$ , of  $\mathcal{E}_\varepsilon$ , by the scalar  $\varepsilon^{2+2\delta} \tau_x \hat{H}_-$  given by (1.15); 2) the limit  $\tau_x \rightarrow 0$  allows to reduce the asymptotic minimization problem to a simpler one where the linear Hamiltonian is exactly  $H_{\ell_V}$  given by (1.16).

One main point in the proof is to have precise energy estimates for the limiting problem. In our case, we obtain them in the limit  $\tau_x \rightarrow 0$ , because explicit calculations are more easily accessible when the magnetic field is constant, that is in the case of  $\mathcal{E}_{H, \min}$ . In theory, if one had precise energy estimates for a general  $\tau_x$  for the intermediate adiabatic model with the linear part  $\hat{H}_-$ , complete results could be performed for general values of  $\tau_x$ .

**Remark 1.4.** The exponent  $\nu_0 = \nu_{\ell_V, G}$  is a Lojasiewicz-Simon exponent (see Remark 4.3 for an explanation and a.e. [Loj, BCR] for the definition of Lojasiewicz exponents and [Sim] for its extension to PDE problems). It is  $\frac{1}{2}$  when the Lagrange multiplier associated with  $u \in \text{Argmin } \mathcal{E}_H$  is a simple eigenvalue of  $\hat{H}_{\ell_V} + G|\psi|^2$ . There are reasons to think that it is the case for generic values  $(\ell_V, G) \in (0, +\infty) \times [0, +\infty)$ , namely outside a subanalytic subset of dimension smaller than 1 (and possibly 0). Nevertheless for  $G = 0$ , there is a discrete set of values of  $\ell_V$  for which  $H_{\ell_V}$  has multiple eigenvalues.

**Consequences and applications:** One issue is whether the presence of vortices (zeroes of the wave function with circulation around them) might break the adiabatic approach. The answer contained in our theorem is that vortices of  $\psi$  in the original problem and vortices of the ground state of the Gross-Pitaevskii energy  $\mathcal{E}_H$  are close and that the minimization of  $\mathcal{E}_H$  provides all the information on the defects of  $\psi$ . Indeed, the smallness of  $a_+$  in  $L^\infty$  indicates that the vortices of  $\psi$  and  $a_-$  are close, and the last estimate of the theorem provides that the vortices of  $a_-$  are close to that of the Gross-Pitaevskii problem.

Numerically, in [GCYRD], the authors observe vortices in a system with artificial gauge as presented in [DGJO] and modeled with the energy  $\mathcal{E}_\varepsilon$ . They check that the vortex pattern is close to that of the Gross-Pitaevskii energy. If one wants to use our results, one may proceed in the following way: once  $G$  is fixed, choose  $\ell_V$  such that the minimizers of  $\mathcal{E}_H$  have vortices (detailed conditions will be given in section 4.2). Then take  $\tau_x > 0$  and  $\varepsilon > 0$  small enough so that the  $L^\infty$  norm of  $a_+$  and the  $L^\infty$  distance from  $\chi(\tau_x^{\frac{1}{9}})a_-$  to a ground state of  $\mathcal{E}_H$  are small. In the above result, the constants are not explicitly controlled and this control is worse and worse when  $\delta$  increases. So it is not explicit for given numerical values of the parameters  $\ell_V, G, \tau_x, \varepsilon$  or equivalently  $\ell_V, G, \kappa, k, \ell_\kappa$ . Nevertheless it provides a framework for numerical simulations, where the observation of vortices can be confirmed by decreasing  $\varepsilon$  and  $\tau_x$ . The parameters of the experiments are just at the border where our constants may become too large to provide a reasonable approximation.

The definitions (1.3) of  $\varepsilon$  and (1.5) of  $\tau_x$ , transform the condition (1.18) into

$$\left(\frac{k^2}{\kappa}\right)^{\frac{2\delta}{1+2\delta}} \ll \left(\frac{1}{k\ell_\kappa}\right)^{\frac{5}{3}}.$$

The larger  $\delta$ , the better, but  $\delta$  must not be too large because of the value of the constants  $C_\delta, C_{\delta, \chi}$ . A value of a few units for  $\delta$  does not affect them too much. Another reason for keeping  $\delta$  small is that the initial small parameter is  $\varepsilon^{2+2\delta}$ , while the final error estimate of  $d_{\mathcal{H}_2}(\chi_1(\tau_x^{\frac{1}{9}})a_-, \text{Argmin } \mathcal{E}_H)$  (or  $d_{L^\infty}(\chi_1(\tau_x^{\frac{1}{9}})a_-, \text{Argmin } \mathcal{E}_H)$ ) contains also an  $\mathcal{O}(\varepsilon)$  term. As an example for  $\delta = \frac{5}{2}$ , the above relation becomes

$$\frac{1}{(k\ell_\kappa)^{7/3}} \gg \frac{k^2}{\kappa} \quad , \quad \tau_x = \frac{1}{k\ell_\kappa} \quad , \quad \varepsilon = \left(\frac{k^2}{\kappa}\right)^{\frac{1}{7}}.$$



A given precision of order  $\varepsilon + \tau_x^{\frac{1}{3}}$ , is more easily achieved by taking  $k$  small and  $\ell_\kappa = \frac{1}{\tau_x k}$  large (for example  $k = 0.1$ ,  $\ell_\kappa = 500 \times 25$  is better than the values  $k = 50$ ,  $\ell_\kappa = 25$  given in the introduction). Note also that the external potential  $V_{\varepsilon, \tau}$ , defined in (1.13) must be adjusted up to the order  $\varepsilon^{2+2\delta} = \frac{k^2}{\kappa}$ .

## 1.2 Gist of the analysis

Following the general idea of the founding articles [BoFo, BoOp] of Born, Fock and Oppenheimer, it is well known in the physics literature that a Hamiltonian system

$$(\varepsilon D_q)^2 + u_0(q) \begin{pmatrix} E_+(q) & 0 \\ 0 & E_-(q) \end{pmatrix} u_0(q)^*$$

is unitarily equivalent to a diagonal Hamiltonian plus a remainder term:

$$\varepsilon^2 \left[ \begin{pmatrix} (D_q - A(q))^2 & 0 \\ 0 & (D_q + A(q))^2 \end{pmatrix} + |X(q)|^2 \right] + R(\varepsilon),$$

where  $(D_{q_i} \mp A_i(q))$  are the covariant derivatives ( $\mp A(q)$  is the adiabatic connection) associated with the fiber bundles  $u_0(q) \begin{pmatrix} \mathbb{C} \\ 0 \end{pmatrix}$  and  $u_0(q) \begin{pmatrix} 0 \\ \mathbb{C} \end{pmatrix}$ , and  $|X(q)|^2$  is the Born-Huang potential.

Since [Kat] and until recently ([NeSo, MaSo, PST, PST2]), this problem has been widely studied by mathematicians, and the remainder term is formally:

$$R(\varepsilon) = \sum_{i,j} \varepsilon^2 C_{ij}(q) (\varepsilon D_{q_i}) (\varepsilon D_{q_j}) + \mathcal{O}(\varepsilon^3).$$

It is smaller than  $\varepsilon^2$  for bounded frequencies (or momenta) but it has the same size as the main term for a typical frequency of order  $\frac{1}{\varepsilon}$ . For a nonlinear problem or without any information about the frequency localization of the quantum states, it is important to estimate the error terms in the low and high frequency regimes.

Introducing  $\delta > 0$  allows to obtain at the formal level

$$\varepsilon^{2+2\delta} \left[ \begin{pmatrix} (D_q - A(q))^2 & 0 \\ 0 & (D_q + A(q))^2 \end{pmatrix} + |X(q)|^2 \right] + \sum_{i,j} \varepsilon^{2+4\delta} C_{ij}(q) (\varepsilon D_{q_i}) (\varepsilon D_{q_j}) + \mathcal{O}(\varepsilon^{3+4\delta}),$$

where the remainder term is now  $\mathcal{O}(\varepsilon^{2+4\delta})$  at the typical frequency  $\frac{1}{\varepsilon}$  and thus  $\mathcal{O}(\varepsilon^{2\delta})$  times the size of the main term. Such an error estimate can be made in the  $L^2$ -sense when applied to some wave function  $\psi$  lying in  $\{|p| \leq r\}$ , with  $p$  quantized into  $\varepsilon D_q$ , or more precisely fulfilling  $\psi = \chi(\varepsilon D_q) \psi$  for some  $\chi \in C_0^\infty(\{|p| \leq 2r\})$  with

$$\|R(\varepsilon)\psi\| \leq C_\chi(\varepsilon^{2+4\delta} + C_N \varepsilon^N) \|\psi\| \leq (C'_{\chi, \delta} \varepsilon^{2\delta}) \varepsilon^{2+2\delta} \|\psi\|.$$

where  $C_N$  essentially depends on the estimates of  $N$ -derivatives of  $u_0(q)$ ,  $E_\pm(q)$ . For a fixed  $\delta$ , we choose  $N \geq 2 + 4\delta$ .

**Remark 1.5.** About the choice  $\delta > 0$ , another strategy could be considered in order to optimize the exponent  $\delta$ , w.r.t  $\varepsilon$ : under analyticity assumptions or more generally assumptions which lead to an explicit control of  $C_N$  in terms of  $N$ , one could think of optimizing first  $C_N \varepsilon^N$  w.r.t to  $N$  according to the methods of [NeSo, Sor, MaSo]. As an example with  $C_N \leq N!$ , this would lead to  $C_N \varepsilon^N \leq C e^{-\frac{1}{\varepsilon}}$  after choosing  $N = N(\varepsilon) = \lceil \frac{1}{\varepsilon} \rceil$ , with some  $C \leq 1$ . Then taking  $\delta = \delta(\varepsilon) = -\frac{1}{4\varepsilon \log(\varepsilon)}$  would lead to

$$CC_\chi(\varepsilon^{2+4\delta(\varepsilon)} + e^{-\frac{1}{\varepsilon}}) \leq 2CC_\chi e^{-\frac{1}{\varepsilon}} \|\psi\|.$$

When  $\delta(\varepsilon) \rightarrow \infty$  and as compared with  $\varepsilon^{2+2\delta(\varepsilon)}$  considered as the order 1 term, an  $\mathcal{O}(\varepsilon^{2+4\delta(\varepsilon)})$  remainder term is almost of order 2.

We do not consider this optimization of  $\delta$  w.r.t  $\varepsilon$ , with  $\lim_{\varepsilon \rightarrow 0} \delta(\varepsilon) = +\infty$ , because our initial small parameter is  $\varepsilon^{2+2\delta}$  and the final result of Theorem 1.2, (the estimate about  $d_{\mathcal{H}_2}(\chi_1(\tau_x^{\frac{1}{2}} \cdot) a_-, \text{Argmin } \mathcal{E}_H)$  in the nonlinear problem), contains an  $\mathcal{O}(\varepsilon)$ . Hence we keep  $\delta > 0$  independent of  $\varepsilon$ . This is why  $\delta$  is still present in the constants of Theorem 1.2.

We need to perform a frequency (or momentum) truncation. We decompose a general  $\psi$  into  $\chi(\varepsilon D_q)\psi + (1 - \chi(\varepsilon D_q))\psi$  and use rough estimates for the part  $(1 - \chi(\varepsilon D_q))\psi$  which will be compensated in the minimization problem for  $\mathcal{E}_\varepsilon$  by good a priori estimates for the norm  $\|(1 - \chi(\varepsilon D_q))\psi\|$  of the high-frequency part. We also have to check that the unitary transform  $\tilde{U}$ , implementing the adiabatic approximation, does not perturb too much the nonlinear part of  $\mathcal{E}_\varepsilon(\psi)$ .

In our case, the limit  $\varepsilon \rightarrow 0$  leads to the Born-Oppenheimer Hamiltonians

$$-\partial_x^2 - (\partial_y \mp \frac{ix}{2\sqrt{1+\tau_x x^2}})^2 + \frac{v(\sqrt{\tau_x} \cdot)}{\ell_V^2 \tau_x},$$

which, in a second step, in the limit  $\tau_x \rightarrow 0$ , leads to  $H_{\ell_V}$  (with the sign  $-ix$  for the lower energy band). This means that the convergence to the Born-Oppenheimer Hamiltonian as  $\varepsilon \rightarrow 0$  has to be uniform w.r.t  $\tau_x \in (0, 1]$ . This last point requires to reconsider carefully the work of [PST] by following the uniformity w.r.t  $\tau$  of the estimates given by Weyl-Hörmander calculus ([Hor, BoLe]) for  $\tau$ -dependent metrics which have uniform structural constants.

This is done for the low frequency part in Section 2 while the basic tools of semiclassical calculus are reviewed and adapted in the Appendix A.

In Section 3 the error associated in the high-frequency part is considered, as well as the effect of the unitary adiabatic transformation on the nonlinear term. Once the adiabatic approximation is well justified in this rather involved framework, the accurate analysis, as well as the comparison when  $\tau_x$  is small, of the two reduced models (the one with  $H_{\ell_V}$  and the one with  $\hat{H}_-$ ) is carried out in Section 4. This follows the general scheme of comparison of minimization problems: 1) Write energy estimates; 2) Use bootstrap arguments and possibly Łojasiewicz-Simon inequalities in order to compare the minimizers in the energy space; 3) Use the Euler-Lagrange equations in order to get a better comparison

in higher regularity spaces.

In Section 5, all the information of the previous sections is gathered in order to prove Theorem 1.2 : existence of a minimizer for  $\mathcal{E}_\varepsilon$  in Proposition 5.3, key energy estimates in Proposition 5.4 and bounds for minimizers in Proposition 5.6. Some comments and additional results are pointed out in Section 6, namely: 1) the question of the smallness condition of  $\varepsilon$  w.r.t  $\tau_x$  appearing in Theorem 1.2; 2) the possible extension to anisotropic nonlinearities (one would have to check that the unitary transform implementing the adiabatic approximation does not perturb the nonlinear part); 3) the minimization problem for excited states, i.e. locally and approximately carried by  $\psi_+$  instead of  $\psi_-$ ; 4) the extension to the problem of the time nonlinear dynamics of adiabatically prepared states.

## 2 Adiabatic approximation for the linear problem

In [PST], the adiabatic approximation is completely justified for bounded symbols or when global elliptic properties of the complete matricial symbol allow to reduce to this case after spectral truncation. Unfortunately, it is not the case here, because the eigenvalues of the symbol of the linear part  $H_{Lin}$  are  $\varepsilon^{2\delta}\tau_x\tau_y|p|^2 + V_{\varepsilon,\tau}(x,y) \pm \Omega(\sqrt{\frac{\tau_x}{\tau_y}}x)$ . In [Sor], the adiabatic theory for unbounded symbols is developed after stopping the complete asymptotic expansion in an optimal way, under some analyticity assumptions, but this would be particularly tricky here with divergences occurring both in the momentum and position directions. We shall see that the sublinear divergence in position makes no difficulty after using the right Weyl-Hörmander class. The quadratic divergence in momentum, with the kinetic energy  $\tau_x\tau_y|p|^2$  is solved by first considering truncated kinetic energies and using the additional scaling factor  $\varepsilon^{2\delta}$ ,  $\delta > 0$ , in front of the kinetic energy term.

Our problem shows an anisotropy in the position variables  $(x,y)$ . The analysis of the linear problem can be treated in  $\mathbb{R}^d$ . Then we split the position and momentum variables,  $q \in \mathbb{R}^d$  and  $p \in \mathbb{R}^d$ , into:

$$q = (q', q'') \quad , \quad p = (p', p'') \quad q', p' \in \mathbb{R}^{d'} \quad , \quad q'', p'' \in \mathbb{R}^{d''} \quad , \quad d' + d'' = d \quad ,$$

and the pair  $(\tau_x, \tau_y)$  is accordingly denoted by  $(\tau', \tau'') \in (0, 1]^2$ .

From this section, some notions and notations related with semiclassical analysis are used. In particular, the notation  $S_u(m_\tau, g_\tau)$  refers to classes of  $(\varepsilon, \tau)$ -dependent symbols of which the seminorms are uniformly controlled w.r.t to the parameters  $(\varepsilon, \tau) \in (0, \varepsilon_0) \times (0, 1]^2$ . For accurate definitions, we refer the reader to appendix A where all the necessary material is reviewed and adapted for our analysis, assuming knowledges about Fréchet spaces and generalized functions.

## 2.1 Born-Oppenheimer Hamiltonian

Consider the Hamiltonian in  $\hat{H}_\varepsilon = H(q, \varepsilon D_q, \varepsilon)$  with the symbol on  $\mathbb{R}_{q,p}^{2d}$

$$\begin{aligned} H(q, p, \varepsilon) &= \varepsilon^{2\delta} \tau' \tau'' |p|^2 \gamma(\tau' \tau'' |p|^2) + \mathcal{V}(q, \tau, \varepsilon) \\ &= \varepsilon^{2\delta} \tau' \tau'' |p|^2 \gamma(\tau' \tau'' |p|^2) + u_0(q, \tau, \varepsilon) \begin{pmatrix} E_+(q, \tau, \varepsilon) & 0 \\ 0 & E_-(q, \tau, \varepsilon) \end{pmatrix} u_0^*(q, \tau, \varepsilon), \end{aligned}$$

with  $\delta > 0$  and  $(\tau', \tau'') \in (0, 1]^2$ . The following properties, with the splitting of variables  $q = (q', q'') \in \mathbb{R}^d$ , are assumed:

$$\begin{aligned} E_\pm &\in S_u\left(\left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle, \frac{\frac{\tau'}{\tau''} dq'^2}{\left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle^2} + \frac{\tau''}{\tau'} dq''^2\right), \\ E_+(q, \tau, \varepsilon) - E_-(q, \tau, \varepsilon) &\geq C^{-1} \left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle, \\ u_0 &= (u_0^*)^{-1} \in S_u\left(1, \frac{\frac{\tau'}{\tau''} dq'^2}{\left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle^2} + \frac{\tau''}{\tau'} dq''^2; \mathcal{M}_2(\mathbb{C})\right), \\ \gamma &\in \mathcal{C}_0^\infty(\mathbb{R}; \mathbb{R}_+) \quad \text{with} \quad \gamma \equiv 1 \in [0, 2r_\gamma^2]. \end{aligned} \tag{2.1}$$

With these assumptions we are able to justify the Born-Oppenheimer adiabatic approximation for  $\delta > 0$ ,  $\tau', \tau'' \in (0, 1]$ . We shall work with the  $\tau$ -dependent metric

$$g_\tau = \frac{\frac{\tau'}{\tau''} dq'^2}{\left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle^2} + \frac{\tau''}{\tau'} dq''^2 + \frac{\tau' \tau'' dp^2}{\left\langle \sqrt{\tau' \tau''} p \right\rangle^2},$$

on the phase-space  $\mathbb{R}_{q,p}^{2d}$ , which is checked to have uniform properties w.r.t  $\tau \in (0, 1]^2$  in Proposition A.9. The exact definition of the parameter dependent Hörmander symbol classes,  $S_u(m, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , is given in Appendix A (see in particular its meaning for  $\tau$ -dependent metrics in Appendix A.4). We shall use the notation

$$S_u\left(\frac{1}{\left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle \left\langle \sqrt{\tau' \tau''} p \right\rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$$

with the meaning of the exponent  $\infty$  being the same as in  $\mathcal{C}^\infty$  of  $\mathcal{O}(\varepsilon^\infty)$ .

**Theorem 2.1.** *There exists a unitary operator  $\hat{U} = U(q, \varepsilon D_q, \tau, \varepsilon)$  with symbol*

$$\begin{aligned} U(q, p, \tau, \varepsilon) &= u_0(q, \tau, \varepsilon) + \varepsilon u_1(q, p, \tau, \varepsilon) + \varepsilon^2 u_2(q, p, \tau, \varepsilon), \\ \varepsilon^{-2\delta} u_{1,2} &\in S_u\left(\frac{1}{\left\langle \sqrt{\frac{\tau'}{\tau''}} q' \right\rangle \left\langle \sqrt{\tau' \tau''} p \right\rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right), \end{aligned}$$

such that

$$\begin{aligned} \hat{U}^* \hat{H} \hat{U} &= \begin{pmatrix} h_{BO,+}(q, \varepsilon D_q, \varepsilon) & 0 \\ 0 & h_{BO,-}(q, \varepsilon D_q, \varepsilon) \end{pmatrix} \\ &\quad + \varepsilon^{2+4\delta} R_1(q, \varepsilon D_q, \tau, \varepsilon) + \varepsilon^{3+2\delta} R_2(q, \varepsilon D_q, \tau, \varepsilon), \end{aligned} \tag{2.2}$$

with  $h_{BO\pm}(q, p, \tau, \varepsilon)$  equal to

$$\begin{aligned} &= \varepsilon^{2\delta} \tau' \tau'' (|p \mp \varepsilon A|^2 + |\varepsilon X|^2) + E_{\pm} \\ &= \varepsilon^{2\delta} \tau' \tau'' \left[ \sum_{k=1}^d (p_k \mp \varepsilon A_k)^2 + |\varepsilon X_k|^2 \right] + E_{\pm}, \end{aligned} \quad (2.3)$$

when  $\sqrt{\tau' \tau''} |p| \leq r_{\gamma}$ , and

$$\begin{pmatrix} +A_k & X_k \\ \bar{X}_k & -A_k \end{pmatrix} = i u_0^* (\partial_{q^k} u_0).$$

The remainder terms satisfy  $R_1, R_2 \in S_u(1, g_{\tau}; \mathcal{M}_2(\mathbb{C}))$  and  $R_2$  vanishes in  $\{\sqrt{\tau' \tau''} |p| \leq r_{\gamma}\}$  and those estimates are uniform w.r.t  $\delta \in (0, \delta_0]$  (and  $\tau \in (0, 1]^2$ ,  $\varepsilon \in (0, \varepsilon_0]$ ).

**Remark 2.2.** • The remainder term is really negligible only for  $\delta > 0$ . This is explained in Subsection 2.4.

- The (Weyl)-quantization of  $\varepsilon^{2\delta} \tau' \tau'' (|p \mp \varepsilon A|^2 + |\varepsilon X|^2) + E_{\pm}$  is nothing but

$$\varepsilon^{2+2\delta} \tau' \tau'' \left[ \sum_{k=1}^d -(\partial_{q^k} \mp i A_k)^2 + |X_k|^2 \right] + E_{\pm}.$$

## 2.2 Second order computations for space adiabatic approximate projections of the reduced Hamiltonian

We shall consider the matricial symbol, on  $\mathbb{R}_{q,p}^{2d}$ ,

$$H(q, p, \tau, \varepsilon) = f_{\varepsilon}(p, \tau) + E_{+}(q, \tau, \varepsilon) \Pi_0(q, \tau, \varepsilon) + E_{-}(q, \tau, \varepsilon) (1 - \Pi_0(q, \tau, \varepsilon))$$

where  $\Pi_0(q, \tau, \varepsilon) = \Pi_0(q, \tau, \varepsilon)^* = \Pi_0(q, \tau, \varepsilon)^2 \in \mathcal{M}_2(\mathbb{C})$ ,  $\gamma, E_{\pm}$  real-valued, with  $\delta \geq 0$  and the following properties:

$$E_{\pm} \in S_u(\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle, g_{q,\tau}) \quad , \quad \Pi_0 \in S_u(1, g_{q,\tau}; \mathcal{M}_2(\mathbb{C})), \quad (2.4)$$

$$\text{with} \quad g_{q,\tau} = \frac{\frac{\tau'}{\tau''} dq'^2}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle^2} + \frac{\tau''}{\tau'} dq''^2,$$

$$E_{+}(q, \tau, \varepsilon) - E_{-}(q, \tau, \varepsilon) \geq C^{-1} \langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle, \quad (2.5)$$

$$f_{\varepsilon}(p, \tau) = \varepsilon^{2\delta} f_1(\sqrt{\tau' \tau''} p) \quad , \quad f_1 \in \mathcal{C}_0^{\infty}(\mathbb{R}^d; \mathbb{R}) \quad , \quad \delta \geq 0.$$

For conciseness, the arguments  $p, q$  and the parameters  $\tau, \varepsilon$ , will often be omitted in  $\partial_p^{\alpha} f_{\varepsilon}(p)$  and  $\partial_q^{\alpha} E_{\pm}(q)$  or  $\partial_q^{\alpha} \Pi_0$ .

According to Appendix A.4, the metric

$$g_{\tau} = g_{q,\tau} + \frac{\tau' \tau'' dp^2}{\langle \sqrt{\tau' \tau''} p \rangle^2} = \frac{\frac{\tau'}{\tau''} dq'^2}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle^2} + \frac{\tau''}{\tau'} dq''^2 + \frac{\tau' \tau'' dp^2}{\langle \sqrt{\tau' \tau''} p \rangle^2}$$

has the gain function

$$\lambda(q, p) = \min \left( \frac{\langle \sqrt{\tau' \tau''} p \rangle \langle \sqrt{\frac{\tau'}{\tau''}} q \rangle}{\tau'}, \frac{\langle \sqrt{\tau' \tau''} p \rangle}{\tau''} \right) \geq \langle \sqrt{\tau' \tau''} p \rangle.$$

The  $\varepsilon$ -quantized version of the symbol  $A_\varepsilon(q, p)$  will be denoted

$$\hat{A} = A(q, \varepsilon D_q).$$

Note that the symbols  $E_+ - E_-$  is elliptic in its class  $S_u(\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle, g_\tau)$ , and

$$\varepsilon^{-2\delta} f_\varepsilon \in S_u\left(\frac{1}{\langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau\right).$$

Our aim is to compute accurately the adiabatic projection  $\Pi^{(n)}(q, p) = \Pi_0(q, \varepsilon) + \varepsilon \Pi_1(q, p, \varepsilon) + \dots + \varepsilon^n \Pi_n(q, p, \varepsilon)$  such that

$$\hat{\Pi}^{(n)} \circ \hat{\Pi}^{(n)} = \hat{\Pi}^{(n)} + \mathcal{O}(\varepsilon^{n+1}) \quad , \quad [\hat{H}, \hat{\Pi}^{(n)}] = \mathcal{O}(\varepsilon^{n+1}).$$

The general theory presented in [PST], tells us that the asymptotic expansion can be pushed up to  $n = \infty$ , but we will do here accurate calculations up to  $n = 2$  (with additional information for  $n = 3$ ) and then discuss the influence of the factor  $\varepsilon^{2\delta}$ . Those are feasible and rather easy because the kinetic energy term and the two-level potential are simple. This allows to reconsider accurately the arguments sketched in [PST] for the Born-Oppenheimer case with all the technical new peculiarities of our example. Note also that in [MaSo2] chapter 10 explicit calculations have been made up to order  $n = 5$  but in the slightly different framework of time-dependent Born-Oppenheimer approximation oriented to polyatomic molecules : no use of the exponent  $\delta > 0$ , no divergence as  $q \rightarrow \infty$  and no ellipticity problem, no extra-parameter  $\tau$  and the techniques are slightly different although still relying on semiclassical calculus.

Like in [PST], [Sor], [MaSo], [MaSo2], the calculations are first done at the symbolic level and we write

$$(A(\varepsilon) = \mathcal{O}_S(\varepsilon^\nu)) \Leftrightarrow (\varepsilon^{-\nu} A \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))) .$$

For a matricial symbol  $A(q, p)$  (possibly depending on  $(\varepsilon, \tau)$ ), it is convenient to introduce the diagonal and off-diagonal parts

$$A^D(q, p) := \Pi_0(q) A(q, p) \Pi_0(q) + (1 - \Pi_0(q)) A(q, p) (1 - \Pi_0(q)) \quad (2.6)$$

$$A^{OD}(q, p) := \Pi_0(q) A(q, p) (1 - \Pi_0(q)) + (1 - \Pi_0(q)) A(q, p) \Pi_0(q), \quad (2.7)$$

where we recall  $\Pi_0(q) = \Pi_0(q, \tau, \varepsilon)$ . Note the equalities

$$(AB)^D = A^D B^D + A^{OD} B^{OD} \quad , \quad (AB)^{OD} = A^D B^{OD} + A^{OD} B^D. \quad (2.8)$$

The “Pauli matrix”

$$\sigma_3(q, \tau, \varepsilon) = 2\Pi_0(q, \tau, \varepsilon) - \text{Id}_{\mathbb{C}^2}, \quad (2.9)$$

will also be used, with the relations

$$\begin{aligned} \sigma_3^2(q) &= \text{Id}_{\mathbb{C}^2}, \quad \sigma_3(q)A^D(q, p)\sigma_3(q) = A^D(q, p), \\ \sigma_3(q)A^{OD}(q, p)\sigma_3(q) &= -A^{OD}(q, p), \\ \sigma_3(q)A^{OD}(q, p) &= \Pi_0(q)A(q, p)(1 - \Pi_0(q)) - (1 - \Pi_0(q))A(q, p)\Pi_0(q). \end{aligned}$$

We are looking for

$$\Pi^{(n)}(q, p, \tau, \varepsilon) = \sum_{j=0}^n \varepsilon^j \Pi_j(q, p, \tau, \varepsilon) \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C})),$$

$$\text{with } \Pi_j \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C})),$$

and such that

$$\Pi^{(n)} \sharp^\varepsilon \Pi^{(n)} - \Pi^{(n)} = \mathcal{O}_S(\varepsilon^{n+1}), \quad (2.10)$$

$$\Pi^{(n)*} = \Pi^{(n)}, \quad (2.11)$$

$$H \sharp^\varepsilon \Pi^{(n)} - \Pi^{(n)} \sharp H = \mathcal{O}_S(\varepsilon^{n+1}). \quad (2.12)$$

Like in [MaSo], [PST], this system is solved by induction by starting from  $\Pi^{(0)}(q, p, \tau, \varepsilon) = \Pi_0(q, \tau, \varepsilon)$ , with

$$G_{n+1} := \varepsilon^{-(n+1)} \left[ \Pi^{(n)} \sharp^\varepsilon \Pi^{(n)} - \Pi^{(n)} \right] \mod \mathcal{O}_S(\varepsilon), \quad (2.13)$$

$$\Pi_{n+1}^D := -\sigma_3 G_{n+1}^D, \quad (2.14)$$

$$\begin{aligned} F_{n+1} &:= \varepsilon^{-(n+1)} \left[ H \sharp^\varepsilon (\Pi^{(n)} + \varepsilon^{n+1} \Pi_{n+1}^D) \right. \\ &\quad \left. - (\Pi^{(n)} + \varepsilon^{n+1} \Pi_{n+1}^D) \sharp^\varepsilon H \right] \mod \mathcal{O}_S(\varepsilon) \\ &= \varepsilon^{-(n+1)} \left[ H \sharp^\varepsilon \Pi^{(n)} - \Pi^{(n)} \sharp^\varepsilon H \right] \mod \mathcal{O}_S(\varepsilon), \end{aligned} \quad (2.15)$$

$$\Pi_{n+1}^{OD} := -\frac{1}{E_+(q) - E_-(q)} \sigma_3 F_{n+1}^{OD} = \frac{1}{E_+(q) - E_-(q)} F_{n+1}^{OD} \sigma_3. \quad (2.16)$$

The general theory says that the principal symbol of  $F_{n+1}$  is off-diagonal,  $F_{n+1} = F_{n+1}^{OD} \mod \mathcal{O}_S(\varepsilon)$ , and  $F_{n+1}$  can be chosen so that

$$F_{n+1} = F_{n+1}^{OD}. \quad (2.17)$$

Below are the computations up to  $n = 2$  in our specific case. In these computations, we shall use Einstein’s summation rule  $s_k t^k = \sum_k s_k t^k$  with the coordinates  $(p_k, q^k)$  or  $(p^k, q_k)$  with  $p^k = p^\ell \delta_{\ell, k} = p_k$  like in the examples

$$|p|^2 = p^k p_k = p_k p_\ell \delta^{\ell, k} = p^k p^\ell \delta_{k, \ell} \quad , \quad (\partial_p f_\varepsilon) \cdot \partial_q = (\partial_{p^k} f_\varepsilon) \delta^{k, \ell} \frac{\partial}{\partial_{q^\ell}} = (\partial_{p_k} f_\varepsilon) \partial_{q^k}.$$

**n = 0:** Start with  $\Pi^{(0)} = \Pi_0(q, \tau, \varepsilon)$  and notice  $\partial_p \Pi_0 \equiv 0$  and  $\partial_q \Pi_0 \equiv (\partial_q \Pi_0)^{OD}$ .  
**n = 1:** Take

$$G_1 = \Pi_0 \circ \Pi_0 - \Pi_0 = 0, \\ \text{and} \quad \Pi_1^D = 0.$$

Next compute

$$\begin{aligned} \varepsilon^{-1} [H \#^\varepsilon \Pi_0(q, \varepsilon) - \Pi_0(q, \varepsilon) \#^\varepsilon H] &= \varepsilon^{-1} [f_\varepsilon \#^\varepsilon \Pi_0(q, \varepsilon) - \Pi_0(q, \varepsilon) \#^\varepsilon f_\varepsilon] \\ &= -i \partial_{p_k} f_\varepsilon \partial_{q^k} \Pi_0 \mod \mathcal{O}_S(\varepsilon), \end{aligned}$$

and take

$$F_1 = -i \partial_{p_k} f_\varepsilon \partial_{q^k} \Pi_0 = -i \partial_{p_k} f_\varepsilon (\partial_{q^k} \Pi_0)^{OD}, \\ \text{and} \quad \Pi^{(1)} = \Pi_0 + \frac{\varepsilon i \partial_{p_k} f_\varepsilon}{E_+ - E_-} \sigma_3 (\partial_{q^k} \Pi_0)^{OD},$$

with

$$\varepsilon^{-2\delta} \Pi_1 = \frac{i \partial_{p_k} f_1}{E_+ - E_-} \sigma_3 (\partial_{q^k} \Pi_0)^{OD} \in S_u \left( \frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C}) \right).$$

**n = 2:** Consider now

$$\begin{aligned} \varepsilon^2 G_2 &= \Pi^{(1)} \#^\varepsilon \Pi^{(1)} - \Pi^{(1)} \mod \mathcal{O}_S(\varepsilon^3) \\ &= \Pi_0 \#^\varepsilon \Pi_0 - \Pi_0 + \varepsilon (\Pi_0 \#^\varepsilon \Pi_1 + \Pi_1 \#^\varepsilon \Pi_0) - \Pi_1 + \varepsilon^2 \Pi_1 \#^\varepsilon \Pi_1 \mod \mathcal{O}_S(\varepsilon^3). \end{aligned}$$

According to (A.3), with  $\Pi_0 \# \Pi_0 = \Pi_0$  and with

$$\Pi_0 \Pi_1 + \Pi_1 \Pi_0 = \Pi_0^D \Pi_1^{OD} + \Pi_1^{OD} \Pi_0^D = \Pi_1,$$

we can take

$$G_2 = \frac{1}{2i} [-\partial_{q^k} \Pi_0 \partial_{p_k} \Pi_1 + \partial_{p_k} \Pi_1 \partial_{q^k} \Pi_0] + \Pi_1^2.$$

The first term  $-\partial_{q^k} \Pi_0 \partial_{p_k} \Pi_1$ , with Einstein's summation rule, equals

$$\begin{aligned} -\partial_{q^k} \Pi_0 \partial_{p_k} \Pi_1 &= -\frac{i \partial_{p_k p_\ell}^2 f_\varepsilon}{(E_+ - E_-)} (\partial_{q^k} \Pi_0)^{OD} \sigma_3 (\partial_{q^\ell} \Pi_0)^{OD} \\ &= \frac{i \partial_{p_k p_\ell}^2 f_\varepsilon}{(E_+ - E_-)} \sigma_3 (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0), \end{aligned}$$

while the second term  $+(\partial_{p_k} \Pi_1) (\partial_{q^k} \Pi_0)$  gives the same result.

The third term  $\Pi_1^2$  is given by

$$\begin{aligned} \Pi_1^2 &= -\frac{(\partial_{p_k} f_\varepsilon)(\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)^2} \sigma_3 (\partial_{q^k} \Pi_0)^{OD} \sigma_3 (\partial_{q^\ell} \Pi_0)^{OD} \\ &= \frac{(\partial_{p_k} f_\varepsilon)(\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)^2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0). \end{aligned}$$



Hence the diagonal second order correction is given by

$$\begin{aligned} (E_+ - E_-)^2 \Pi_2^D &= -(E_+ - E_-)^2 \sigma_3 G_2 \\ &= -[(\partial_{p_k} f_\varepsilon)(\partial_{p_\ell} f_\varepsilon) + (E_+ - E_-)(\partial_{p_k p_\ell}^2 f_\varepsilon) \sigma_3] (\partial_{q^k} \Pi_0)(\partial_{q^\ell} \Pi_0) \end{aligned}$$

and satisfies

$$\varepsilon^{-2\delta} \Pi_2^D \in S_u \left( \frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C}) \right).$$

Consider now  $\Pi_2^{OD}$ : By referring to (2.17),  $F_2$  can be chosen as the off-diagonal part of  $\varepsilon^{-2} [H \sharp^\varepsilon \Pi^{(1)} - \Pi^{(1)} \sharp^\varepsilon H]$  which, according to the previous steps and (A.3), equals

$$\begin{aligned} & -\frac{1}{8} \left[ \partial_{p_k, p_\ell}^2 H \partial_{q^k, q^\ell}^2 \Pi_0 - \partial_{q^k, q^\ell}^2 \Pi_0 \partial_{p_k, p_\ell}^2 H \right] \\ & + \frac{1}{2i} \left[ \partial_{p_k} H \partial_{q^k} \Pi_1 - \partial_{q^k} H \partial_{p_k} \Pi_1 - \partial_{p_k} \Pi_1 \partial_{q^k} H + \partial_{q^k} \Pi_1 \partial_{p_k} H \right] \mod \mathcal{O}_S(\varepsilon). \end{aligned} \quad (2.18)$$

Since  $\partial_{p_k, p_\ell}^2 H = (\partial_{p_k, p_\ell}^2 f_\varepsilon)$  as a scalar symbol commutes with  $\partial_{q^k q^\ell}^2 \Pi_0$ , the first term of (2.18) vanishes.

Similarly the factor  $\partial_{q^k} \Pi_1$  appearing in the second term of (2.18) contains three terms

$$\begin{aligned} \partial_{q^k} \Pi_1 &= -i \frac{\partial_{q^k} (E_+ - E_-)}{(E_+ - E_-)^2} \sigma_3 (\partial_{p_\ell} f_\varepsilon) (\partial_{q^\ell} \Pi_0) + \frac{i(\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)} (\partial_{q^k} \sigma_3) (\partial_{q^\ell} \Pi_0) \\ &\quad + \frac{i(\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)} \sigma_3 (\partial_{q^k q^\ell}^2 \Pi_0), \end{aligned}$$

where the second one is diagonal (Remember  $\sigma_3(q, \tau, \varepsilon) = 2\Pi_0(q, \tau, \varepsilon) - \text{Id}_{\mathbb{C}^2}$ ). Since  $\partial_{p_k} H = \partial_{p_k} f_\varepsilon$  is diagonal, we get

$$\begin{aligned} & \frac{1}{2i} \left[ \partial_{p_k} H \partial_{q^k} \Pi_1 + \partial_{q^k} \Pi_1 \partial_{p_k} H \right]^{OD} \\ &= (\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon) \sigma_3 \left( \partial_{q^k} [(E_+ - E_-)^{-1} \partial_{q^\ell} \Pi_0] \right)^{OD}. \end{aligned}$$

In the quantity  $-\partial_{q^k} H \partial_{p_k} \Pi_1 - \partial_{p_k} \Pi_1 \partial_{q^k} H$ , the derivatives

$$\partial_{p_k} \Pi_1 = \frac{i(\partial_{p_k p_\ell}^2 f_\varepsilon)}{(E_+ - E_-)} \sigma_3 (\partial_{q^\ell} \Pi_0)^{OD}$$

are off-diagonal factors, while

$$\partial_{q^k} H = (\partial_{q^k} E_+) \Pi_0 + (\partial_{q^k} E_-) (1 - \Pi_0) + (E_+ - E_-) (\partial_{q^k} \Pi_0)^{OD}.$$

With the two equalities,

$$\begin{aligned} & (\partial_{q^k} E_+) \Pi_0 \sigma_3 (\partial_{q^\ell} \Pi_0) + \sigma_3 (\partial_{q^\ell} \Pi_0) (\partial_{q^k} E_+) \Pi_0 = (\partial_{q^k} E_+) \sigma_3 (\partial_{q^\ell} \Pi_0), \\ & (\partial_{q^k} E_-) (1 - \Pi_0) \sigma_3 (\partial_{q^\ell} \Pi_0) + \sigma_3 (\partial_{q^\ell} \Pi_0) (\partial_{q^k} E_-) (1 - \Pi_0) = (\partial_{q^k} E_-) \sigma_3 (\partial_{q^\ell} \Pi_0), \end{aligned}$$

we get

$$-\frac{1}{2i} [\partial_{q^k} H \partial_{p_k} \Pi_1 + \partial_{p_k} \Pi_1 \partial_{q^k} H]^{OD} = -\frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2(E_+ - E_-)} (\partial_{q^k} (E_+ + E_-)) \sigma_3 (\partial_{q^\ell} \Pi_0).$$

This leads to

$$F_2 = (\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon) \sigma_3 (\partial_{q^k} [(E_+ - E_-)^{-1} \partial_{q^\ell} \Pi_0])^{OD} \\ - \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{(E_+ - E_-)} (\partial_{q^k} (E_+ + E_-)) \sigma_3 (\partial_{q^\ell} \Pi_0).$$

and

$$\Pi_2^{OD} = -\frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)} (\partial_{q^k} [(E_+ - E_-)^{-1} \partial_{q^\ell} \Pi_0])^{OD} \\ + \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2(E_+ - E_-)^2} (\partial_{q^k} (E_+ + E_-)) (\partial_{q^\ell} \Pi_0),$$

with

$$\varepsilon^{-2\delta} \Pi_2^{OD} \in S_u \left( \frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C}) \right).$$

We have almost proved the

**Proposition 2.3.** *The pseudodifferential operator  $\hat{\Pi}(\varepsilon) = \hat{\Pi}(q, \varepsilon D_q, \varepsilon)$  given by*

$$\Pi(q, p, \varepsilon) = \Pi_0(q, \varepsilon) + \varepsilon \Pi_1(q, p, \varepsilon) + \varepsilon^2 \Pi_2(q, p, \varepsilon)$$

$$\text{with } \Pi_1(q, p, \varepsilon) = \Pi_1(q, p, \varepsilon)^{OD} = \frac{i \partial_{p_k} f_\varepsilon}{(E_+ - E_-)} \sigma_3 (\partial_{q^k} \Pi_0),$$

$$\Pi_2(q, p, \varepsilon) = \Pi_2(q, p, \varepsilon)^D + \Pi_2(q, p, \varepsilon)^{OD},$$

$$\Pi_2(q, p, \varepsilon)^D = -\frac{1}{(E_+ - E_-)^2} [(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon) \\ + (E_+ - E_-) (\partial_{p_k p_\ell}^2 f_\varepsilon)] (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0),$$

$$\Pi_2(q, p, \varepsilon)^{OD} = -\frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)} (\partial_{q^k} [(E_+ - E_-)^{-1} \partial_{q^\ell} \Pi_0])^{OD} \\ + 2 \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{(E_+ - E_-)^3} (\partial_{q^k} (E_+ + E_-)) (\partial_{q^\ell} \Pi_0),$$

$$\text{and } \varepsilon^{-2\delta} \Pi_1, \varepsilon^{-2\delta} \Pi_2 \in S_u \left( \frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C}) \right),$$

satisfies

$$\hat{\Pi} \circ \hat{\Pi} = \hat{\Pi} + \mathcal{O}(\varepsilon^{3+2\delta}) \quad , \quad \hat{\Pi}^* = \hat{\Pi} \quad , \quad [\hat{H}, \hat{\Pi}] = \mathcal{O}(\varepsilon^{3+2\delta}),$$

in  $\mathcal{L}(L^2(\mathbb{R}^d; \mathbb{C}^2))$ . Moreover the estimates in  $\mathcal{L}(L^2(\mathbb{R}^d; \mathbb{C}^2))$  of the remainder terms do not depend on the parameter  $\tau = (\tau', \tau'') \in (0, 1]^2$  and  $\delta > 0$ , as soon as  $\varepsilon \in (0, \varepsilon_0)$ .

**Proof:** The above construction gives immediately

$$\hat{\Pi} \circ \hat{\Pi} = \hat{\Pi} + \mathcal{O}(\varepsilon^3) \quad , \quad \hat{\Pi}^* = \hat{\Pi} \quad , \quad [\hat{H}, \hat{\Pi}] = \mathcal{O}(\varepsilon^3) ,$$

The first improved estimates come from the fact that

$$\hat{\Pi} \circ \hat{\Pi} - \hat{\Pi}$$

contains only terms which are Moyal products with a  $\Pi_1$  or a  $\Pi_2$  factor, with cancellations up to the  $\varepsilon^2$  coefficient. Both of them have seminorms of order  $\varepsilon^{2\delta}$ .

For the last one, this is a similar argument after decomposing

$$[\hat{H}, \hat{\Pi}] = [\varepsilon^{2\delta} f_1(\sqrt{\tau' \tau''} \varepsilon D_q), \hat{\Pi}_0] + [\hat{H}, \varepsilon \hat{\Pi}_1 + \varepsilon^2 \hat{\Pi}_2] .$$

□

The above result can be improved after considering what happens at step  $n = 3$  when  $f_{\varepsilon, \tau}(p) = \varepsilon^{2\delta} f_1(\sqrt{\tau' \tau''} p)$  is at most quadratic w.r.t  $p$  in some region. Before this, let us examine the remainders of order 3 in  $\varepsilon$ .

**n = 3 :** The remainder term

$$\begin{aligned} \varepsilon^3 G_3 &= \Pi^{(2)} \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \\ &= \varepsilon (\Pi_0 \sharp^\varepsilon \Pi_1 + \Pi_1 \sharp^\varepsilon \Pi_0 - \Pi_1) + \varepsilon^2 (\Pi_1 \sharp^\varepsilon \Pi_1 + \Pi_0 \sharp^\varepsilon \Pi_2 + \Pi_2 \sharp^\varepsilon \Pi_0 - \Pi_2) \\ &\quad + \varepsilon^3 (\Pi_1 \sharp^\varepsilon \Pi_2 + \Pi_2 \sharp^\varepsilon \Pi_1) + \varepsilon^4 \Pi_2 \sharp^\varepsilon \Pi_2 . \end{aligned}$$

Using the construction of  $\Pi_1$  and  $\Pi_2$  and the fact that  $\varepsilon^{-2\delta} \Pi_1$  and  $\varepsilon^{-2\delta} \Pi_2$  belong to  $S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''} q'} \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ , the expansion of the Moyal product (A.2)-(A.3) tells us

$$\Pi^{(2)} \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} = \varepsilon^3 [A_G(\partial_q^2 \Pi_0, \partial_p^2 \Pi_1, \varepsilon) + B_G(\partial_q \Pi_0, \partial_p \Pi_2, \varepsilon)] + \varepsilon^{3+4\delta} R_G \quad (2.19)$$

where  $R_G \in S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''} q'} \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$  and  $A_G(., \varepsilon)$ ,  $B_G(., \varepsilon)$  have an asymptotic expansion in terms of  $\varepsilon$ , of which all the terms are bilinear differential expressions of their arguments. For the commutator with  $\hat{H}$ , write

$$\begin{aligned} [H \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \sharp^\varepsilon H] &= [f_\varepsilon(p) \sharp^\varepsilon \Pi_0(q) - \Pi_0(q) \sharp^\varepsilon f_\varepsilon(p)] \\ &\quad + [f_\varepsilon(p) \sharp^\varepsilon (\varepsilon \Pi_1 + \varepsilon^2 \Pi_2) - (\varepsilon \Pi_1 + \varepsilon^2 \Pi_2) \sharp^\varepsilon f_\varepsilon(p)] \\ &\quad + [(E_+ \Pi_0 + E_- (1 - \Pi_0)) \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \sharp^\varepsilon (E_+ \Pi_0 + E_- (1 - \Pi_0))] \end{aligned}$$

After eliminating all the terms which are cancelled while constructing  $\Pi_1$  and  $\Pi_2$ , the contributions of all three terms of the right-hand side can be analyzed. The contribution of the third term is similar to what we got for  $G_3$ :

$$\varepsilon^3 [A_H(\partial_q^2 (E_\pm \Pi_0), \partial_p^2 \Pi_1, \varepsilon) + B_H(\partial_q (E_\pm \Pi_0), \partial_p \Pi_2, \varepsilon)] + \varepsilon^{3+4\delta} R_{H,1}$$

with  $R_{H,1} \in S_u\left(\frac{1}{\langle \sqrt{\tau'\tau''}p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ . With the uniform estimate of  $\varepsilon^{-2\delta}\Pi_1$ ,  $\varepsilon^{-2\delta}\Pi_2$  and  $\varepsilon^{-2\delta}f_\varepsilon$ , the contribution of the second term is estimated as  $\varepsilon^{3+4\delta}R_{H,2}$  with  $R_{H,2} \in S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}q'} \rangle \langle \sqrt{\tau'\tau''}p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ . The contribution of the first term is  $\varepsilon^3 C_H(\partial_p^3 f_\varepsilon, \partial_q^3 \Pi_0, \varepsilon)$  and we get

$$\begin{aligned} \left[ H \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \sharp^\varepsilon H \right] &= \varepsilon^3 \left[ C_H(\partial_p^3 f_\varepsilon, \partial_q^3 \Pi_0, \varepsilon) + \right. \\ &\quad \left. A_H(\partial_q^2(E_\pm \Pi_0), \partial_p^2 \Pi_1, \varepsilon) + B_H(\partial_q(E_\pm \Pi_0), \partial_p \Pi_2, \varepsilon) \right] + \varepsilon^{3+4\delta} R_H \end{aligned} \quad (2.20)$$

where the expansions of  $A_H$ ,  $B_H$  and  $C_H$  w.r.t to  $\varepsilon$  have terms which are bilinear differential expression of their arguments, and the remainder  $R_H$  belongs to  $S_u\left(\frac{1}{\langle \sqrt{\tau'\tau''}p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ .

**Proposition 2.4.** *With  $f_\varepsilon(p) = \varepsilon^{2\delta} f_1(\sqrt{\tau'\tau''}p)$ , assume that the third differential  $\partial_p^3 f_1$  vanishes in  $\{|p| \leq r\}$  and fix  $r' \in (0, r)$ . Then the remainders of Proposition 2.3 equal*

$$\hat{\Pi} \circ \hat{\Pi} - \hat{\Pi} = \varepsilon^{3+2\delta} \hat{R}_{G,1} + \varepsilon^{3+4\delta} \hat{R}_{G,2} \quad (2.21)$$

$$[\hat{H}, \hat{\Pi}] = \varepsilon^{3+2\delta} \hat{R}_{H,1} + \varepsilon^{3+4\delta} \hat{R}_{H,2} \quad (2.22)$$

where  $R_{G,1 \text{ or } 2}$  belong to  $OpS_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}q'} \rangle \langle \sqrt{\tau'\tau''}p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ ,  $R_{H,1 \text{ or } 2}$  belong to  $OpS_u\left(\frac{1}{\langle \sqrt{\tau'\tau''}p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$  and  $R_{G \text{ or } H,1} \equiv 0$  in  $\left\{|\sqrt{\tau'\tau''}p| < r'\right\}$ . Those estimates are uniform for  $\tau \in (0, 1]^2$ ,  $\delta \in [0, \delta_0]$  and  $\varepsilon \in (0, \varepsilon_0)$ .

**Proof:** After noticing that the symbol  $\Pi_1$  is a linear expression in  $\partial_p f_\varepsilon$  while the symbol  $\Pi_2$  is the sum of a linear expression of  $\partial_p^2 f_\varepsilon$  and quadratic expression in  $\partial_p f_\varepsilon$ , the identities (2.19) and (2.20) imply

$$\begin{aligned} \Pi^{(2)} \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} &= \varepsilon^{3+2\delta+N} R_N + \varepsilon^{3+4\delta} R_G, \\ \left[ H \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \sharp^\varepsilon H \right] &= \varepsilon^{3+2\delta+N} R_N + \varepsilon^{3+4\delta} R_H, \end{aligned}$$

for an arbitrary large  $N \in \mathbb{N}$ , in  $\left\{|\sqrt{\tau'\tau''}p| < r\right\}$ . Choose<sup>1</sup>  $N \geq 2\delta$  and take a cut-off function  $\chi \in \mathcal{C}_0^\infty(\{|p| < r\})$  such that  $\chi \equiv 1$  in a neighborhood  $\{|p| \leq r'\}$ . Writing for the symbol

$$S = \Pi^{(2)} \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \quad \text{or} \quad S = \left[ H \sharp^\varepsilon \Pi^{(2)} - \Pi^{(2)} \sharp^\varepsilon H \right],$$

$$S = S \times \chi(\sqrt{\tau'\tau''}p) + S \times (1 - \chi(\sqrt{\tau'\tau''}p)),$$

yields the result.  $\square$

---

<sup>1</sup>Here the estimates become  $\delta$ -dependent, because a large  $\delta$  requires a large  $N$ . It is uniformly controlled when  $\delta \leq \delta_0$ .

### 2.3 Unitaries and effective Hamiltonian

We strengthen a little bit the assumptions (2.4)-(2.5), with the condition

$$\begin{aligned} \Pi_0(q, \tau, \varepsilon) &= u_0(q, \tau, \varepsilon) P_+ u_0(q, \tau, \varepsilon)^* \\ \text{with } P_+ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad u_0 = (u_0^*)^{-1} \in S(1, g_{q, \tau}; \mathcal{M}_2(\mathbb{C})), \end{aligned} \quad (2.23)$$

fulfilled in our example. The operator  $\hat{u}_0$  is nothing but the local unitary transformation  $u_0(q, \tau)$ , on  $L^2(\mathbb{R}^d; \mathbb{C}^2)$ .

With the approximate projection  $\hat{\Pi} = \hat{\Pi}(q, \varepsilon D_q, \tau, \varepsilon)$  given in Proposition 2.3, Proposition A.5 tells us that a true orthogonal projection  $\hat{P}$  can be associated when  $\varepsilon_0$  is chosen small enough, by taking

$$\hat{P} = \frac{1}{2i\pi} \int_{|z-1|=1/2} (z - \hat{\Pi})^{-1} dz, \quad (2.24)$$

with

$$\hat{P} = P(q, \varepsilon D_q, \tau, \varepsilon) \quad , \quad P \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C})), \quad (2.25)$$

$$P(q, p, \tau, \varepsilon) - \Pi(q, p, \tau, \varepsilon) = \varepsilon^{3+2\delta} R_1(q, p, \tau, \varepsilon) + \varepsilon^{3+4\delta} R_2(q, p, \tau, \varepsilon), \quad (2.26)$$

$$\text{with } R_1, R_2 \in S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} q' \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right),$$

$$\hat{P} \circ \hat{P} = \hat{P} = \hat{P}^*,$$

$$[\hat{H}, \hat{P}] = \varepsilon^{3+2\delta} \hat{C}_1(\tau, \varepsilon) + \varepsilon^{3+4\delta} \hat{C}_2(\tau, \varepsilon), \quad (2.27)$$

$$\text{with } C_1, C_2 \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C})),$$

$$\text{and } \left\| \hat{P} - \hat{u}_0 P_+ \hat{u}_0^* \right\|_{\mathcal{L}(L^2)} \leq C\varepsilon. \quad (2.28)$$

For a general  $f_1 \in \mathcal{C}_0^\infty$ ,  $R_2$  and  $C_2$  are included in the main remainder term. When  $f_1$  is quadratic in  $\{|p| < r\}$ , then one can assume that  $R_1$  and  $C_1$  vanishes in  $\left\{ \sqrt{\tau' \tau''} |p| < r' \right\}$  for  $r' < r$ , according to Proposition 2.4 and Proposition A.5

Instead of constructing unitaries between  $\hat{P}(\tau, \varepsilon)$  and  $P_+$  by the induction presented in [PST] and similar to (2.13), (2.14), (2.15), (2.16), we use like in [MaSo] Nagy's formula ([NeSo], [MaSo], [PST])

$$\begin{aligned} P_2 &= W P_1 W^* \quad , \quad W^* W = W W^* = 1, \\ \text{with } W &= (1 - (P_2 - P_1)^2)^{-1/2} [P_2 P_1 + (1 - P_2)(1 - P_1)] \quad , \quad (2.29) \\ \text{when } P_j &= P_j^2 = P_j^* \quad \text{for } j = 1, 2, \quad \text{and } \|P_2 - P_1\|_{\mathcal{L}} < 1, \end{aligned}$$

easier to handle for direct second order computations in our case.

**Proposition 2.5.** *With the definitions (2.23) and (2.24) after Proposition 2.3, there exists a unitary operator  $\hat{U}$  on  $L^2(\mathbb{R}; \mathbb{C}^2)$  such that*

$$\begin{aligned} \hat{P} &= \hat{U} P_+ \hat{U}^*, \\ \hat{U} &= U(q, \varepsilon D_q, \tau, \varepsilon) \quad , \quad U \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C})), \\ \text{with} \quad U(q, p, \tau, \varepsilon) &= u_0(q, \tau, \varepsilon) + \varepsilon u_1(q, p, \tau, \varepsilon) + \varepsilon^2 u_2(q, p, \tau, \varepsilon), \\ u_1(q, p, \varepsilon) &= -\frac{i \partial_{p_k} f_\varepsilon}{(E_+ - E_-)} (\partial_{q^k} \Pi_0) u_0, \\ \text{and} \quad \varepsilon^{-2\delta} u_1, \varepsilon^{-2\delta} u_2 &\in S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right). \end{aligned}$$

Moreover, when  $f_1$  is a quadratic function in  $\{|p| < r\}$  and  $r'$  is fixed in  $(0, r)$ , the term  $u_2$  can be decomposed into

$$u_2(q, p, \tau, \varepsilon) = \varepsilon^{2\delta} v_2(q, p, \tau, \varepsilon) + \varepsilon^{4\delta} \tilde{v}_2(q, p, \tau, \varepsilon)$$

where  $v_2$  does not depend on  $p$  in  $\left\{ \sqrt{\tau' \tau''} |p| < r' \right\}$  and  $v_2, \tilde{v}_2$  belong to the symbol class  $S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ .

**Proof:** The notation  $\hat{R}$  will denote a generic remainder term of the form  $\hat{R} = R(q, \varepsilon D_q, \tau, \varepsilon)$  with  $R \in S_u\left(\frac{1}{\langle \sqrt{\frac{\tau'}{\tau''}} \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ . The notation  $\underline{\hat{R}}$  is used for a symbol  $\underline{R}$ , like  $R$  but which vanishes around  $\left\{ \sqrt{\tau' \tau''} |p| < r' \right\}$ . We apply Nagy's formula (2.29) with  $P_1 = \hat{u}_0 P_+ \hat{u}_0^* = \Pi_0(q, \tau, \varepsilon)$  and  $P_2 = \hat{P}(\tau, \varepsilon)$  with

$$\hat{P} = \Pi_0(q, \tau, \varepsilon) + \varepsilon \Pi_1(q, \varepsilon D_q, \tau, \varepsilon) + \varepsilon^2 \Pi_2(q, \varepsilon D_q, \tau, \varepsilon) + \varepsilon^{3+2\delta} \underline{\hat{R}} + \varepsilon^{3+4\delta} \hat{R}.$$

In the expression of  $\hat{W}(\varepsilon)$  given by (2.29), the first factor is nothing but

$$(1 - (\hat{P} - \Pi_0(q, \tau, \varepsilon))^2)^{-1/2} = 1 + \frac{\varepsilon^2}{2} (\Pi_1)^2(q, \varepsilon D_q, \tau, \varepsilon) + \varepsilon^{3+4\delta} \hat{R},$$

owing to  $P - \Pi_0 = \mathcal{O}_S(\varepsilon^{2\delta})$ . In the factor  $[P_2 P_1 + (1 - P_2)(1 - P_1)]$ , the first term equals

$$\begin{aligned} \hat{P} \circ \Pi_0(q, \varepsilon) &= \Pi_0(q, \varepsilon) + \varepsilon \Pi_1(q, \varepsilon D_q, \tau, \varepsilon) \circ \Pi_0(q, \tau, \varepsilon) \\ &\quad + \varepsilon^2 \Pi_2(q, \varepsilon D_q, \tau, \varepsilon) \circ \Pi_0(q, \tau, \varepsilon) + \varepsilon^{3+2\delta} \underline{\hat{R}} + \varepsilon^{3+4\delta} \hat{R}, \end{aligned}$$

while the second term is

$$\begin{aligned} (1 - \hat{P}) \circ (1 - \Pi_0(q, \tau, \varepsilon)) &= (1 - \Pi_0(q, \tau, \varepsilon)) - \varepsilon \Pi_1(q, \varepsilon D_q, \tau, \varepsilon) \circ (1 - \Pi_0(q, \tau, \varepsilon)) \\ &\quad - \varepsilon^2 \Pi_2(q, \varepsilon D_q, \tau, \varepsilon) \circ (1 - \Pi_0(q, \tau, \varepsilon)) + \varepsilon^{3+2\delta} \underline{\hat{R}} + \varepsilon^{3+4\delta} \hat{R}. \end{aligned}$$

Hence we get

$$\begin{aligned}\hat{W} &= [P_2 P_1 + (1 - P_2)(1 - P_1)] = 1 + \varepsilon \Pi_1(q, \varepsilon D_q, \tau, \varepsilon) \circ \sigma_3(q, \tau) \\ &\quad + \varepsilon^2 \Pi_2(q, \varepsilon D_q, \tau, \varepsilon) \circ \sigma_3(q, \tau) + \varepsilon^{3+2\delta} \hat{\underline{R}} + \varepsilon^{3+4\delta} \hat{R}.\end{aligned}$$

The operator  $\hat{U}(\varepsilon)$  is given by  $\hat{U}(\varepsilon) = \hat{W}(\varepsilon) \circ \hat{u}_0$ . The semiclassical calculus recalled in (A.2)-(A.3) yields the result. In the decomposition of  $u_2$ , when  $f_1$  is quadratic around 0, the terms which are linear in  $\varepsilon^{2\delta}$  come with the second derivative of  $f_\varepsilon$ , which does not depend on  $p$ .  $\square$

**Proposition 2.6.** *Introduce the notation for  $k \in \{1, \dots, d\}$*

$$u_0^*(\partial_{q^k} u_0) = -i \begin{pmatrix} A_k & X_k \\ \overline{X_k} & -A_k \end{pmatrix}.$$

*If  $\hat{U}$  is the unitary operator introduced in Proposition 2.5, the conjugated Hamiltonian  $\hat{U}(\varepsilon)^* \hat{H}(\varepsilon) \hat{U}(\varepsilon)$  equals*

$$\hat{U}^* \hat{H} \hat{U} = \begin{pmatrix} \hat{h}_+ & 0 \\ 0 & \hat{h}_- \end{pmatrix} + \varepsilon^{3+2\delta} \hat{R}_1 + \varepsilon^{3+4\delta} \hat{R}_2 \quad (2.30)$$

where the remainder terms  $\hat{R}_{1,2} = R_{1,2}(q, \varepsilon D_q, \tau, \varepsilon)$  belong to  $OpS_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$  and additionally  $R_1 \equiv 0$  in  $\left\{ \sqrt{\tau' \tau''} |p| < r' \right\}$  when  $f_1$  is quadratic in  $\{|p| < r\}$ , with  $r' < r$ .

The symbol  $h_+$  and  $h_-$  are given by

$$\begin{aligned}h_+ &= f_\varepsilon(p) + E_+(q) - \varepsilon(\partial_p f_\varepsilon) \cdot A + \frac{\varepsilon^2}{2} (\partial_{p_k p_\ell}^2 f_\varepsilon) A_k A_\ell \\ &\quad + \frac{\varepsilon^2 (\partial_{p_k p_\ell}^2 f_\varepsilon)}{2} X_k \overline{X}_\ell + \frac{\varepsilon^2 (\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} X_k \overline{X}_\ell, \quad (2.31)\end{aligned}$$

$$\begin{aligned}h_- &= f_\varepsilon(p) + E_-(q) + \varepsilon(\partial_p f_\varepsilon) \cdot A + \frac{\varepsilon^2}{2} (\partial_{p_k p_\ell}^2 f_\varepsilon) A_k A_\ell \\ &\quad + \frac{\varepsilon^2 (\partial_{p_k p_\ell}^2 f_\varepsilon)}{2} \overline{X_k} X_\ell - \frac{\varepsilon^2 (\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} \overline{X_k} X_\ell. \quad (2.32)\end{aligned}$$

**Proof:** From the semiclassical calculus, we already know that  $\hat{U}^* \hat{H} \hat{U}$  is a semiclassical operator with a symbol in  $S_u(\langle \sqrt{\frac{\tau'}{\tau''}} q', g_\tau; \mathcal{M}_2(\mathbb{C}) \rangle)$ . Its off-diagonal part equals

$$\begin{aligned}(1 - P_+) \hat{U}^* \hat{H} \hat{U} P_+ &+ P_+ \hat{U}^* \hat{H} \hat{U} (1 - P_+) \\ &= \hat{U} \left[ \hat{P}, \left[ \hat{P}, \hat{H} \right] \right] \hat{U}.\end{aligned}$$

The almost diagonal form (2.30) of  $\hat{U}^* \hat{H} \hat{U}$  is then a consequence of (2.27). For the second result, it is necessary to compute the diagonal part of the symbol

$U^* \sharp^\varepsilon H \sharp^\varepsilon U$  up to  $\mathcal{O}(\varepsilon^{3+2\delta})$  in  $S_u(1, g_\tau; \mathcal{M}_2)$ . Let us compute the diagonal part of

$$\mathcal{B} := (u_0^* + \varepsilon u_1^* + \varepsilon^2 u_2^*) \sharp^\varepsilon H \sharp^\varepsilon (u_0 + \varepsilon u_1 + \varepsilon^2 u_2),$$

or equivalently  $(u_0 \mathcal{B} u_0^*)^D$  with our notations.

Since  $u_0 = u_0(q, \tau, \varepsilon)$  and  $H = \varepsilon^{2\delta} f_1(\sqrt{\tau' \tau''} p) + \mathcal{V}(q, \tau, \varepsilon)$ , the first Moyal product equals according to (A.2)-(A.3),

$$\begin{aligned} (u_0^* + \varepsilon u_1^* + \varepsilon^2 u_2^*) \sharp^\varepsilon H &= u_0^* H + \varepsilon u_1^* H + \varepsilon^2 u_2^* H \\ &+ \frac{\varepsilon}{2i} \{u_0^*, H\} + \frac{\varepsilon^2}{2i} \{u_1^*, H\} - \frac{\varepsilon^2}{8} (\partial_{q^k q^\ell}^2 u_0^*) (\partial_{p_k p_\ell}^2 H) + \varepsilon^{3+2\delta} R \\ &= u_0^* H + \varepsilon \left[ u_1^* H - \frac{\partial_{p_k} f_\varepsilon}{2i} \partial_{q^k} u_0^* \right] + \varepsilon^2 \left[ u_2^* H + \frac{1}{2i} \{u_1^*, H\} \right. \\ &\quad \left. - \frac{1}{8} (\partial_{q^k q^\ell}^2 u_0^*) (\partial_{p_k p_\ell}^2 f_\varepsilon) \right] + \varepsilon^{3+2\delta} \underline{R} + \varepsilon^{3+4\delta} R, \end{aligned}$$

where  $R$  and  $\underline{R}$  denote generic element of  $S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , with the additional property that  $\underline{R}$  vanishes in  $\{\sqrt{\tau' \tau''} |p| < r'\}$  when  $f_1$  is quadratic in  $\{|p| \leq r\}$  with  $r' < r$ . The reason for the possible decomposition of the remainder, comes again from the fact that the third order remainder term, proportional to  $\varepsilon^{3+2\delta}$ , arises with the third derivative of  $f_\varepsilon$ , the second derivative w.r.t  $p$  of  $u_1$  and the first derivative w.r.t  $p$  of  $u_2$ .

In the same way, the complete expression of  $\mathcal{B}$  is given by

$$\begin{aligned} \mathcal{B}(\varepsilon) &= u_0^* H u_0 + \varepsilon \left[ u_0^* H u_1 + u_1^* H u_0 - \frac{(\partial_{p_k} f_\varepsilon)}{2i} (\partial_{q^k} u_0^*) u_0 + \frac{(\partial_{p_k} f_\varepsilon)}{2i} u_0^* (\partial_{q^k} u_0) \right] \\ &+ \varepsilon^2 \left[ u_2^* H u_0 + u_0^* H u_2 + \frac{1}{2i} \{u_0^*, H, u_1\} + \frac{1}{2i} \{u_1^*, H, u_0\} + \frac{1}{4} \{(\partial_{p_k} f_\varepsilon)(\partial_{q^k} u_0^*), u_0\} \right. \\ &\quad \left. + u_1^* H u_1 - \frac{(\partial_{p_k} f_\varepsilon)}{2i} (\partial_{q^k} u_0^*) u_1 + \frac{1}{2i} \{u_1^*, H\} u_0 \right. \\ &\quad \left. - \frac{1}{8} (\partial_{q^k q^\ell}^2 u_0^*) (\partial_{p_k p_\ell}^2 f_\varepsilon) u_0 - \frac{1}{8} u_0^* (\partial_{p_k p_\ell}^2 f_\varepsilon) (\partial_{q^k q^\ell}^2 u_0) \right] + \varepsilon^{3+2\delta} \underline{R} + \varepsilon^{3+4\delta} R. \end{aligned}$$

By recalling that  $(u_1 u_0^*)^D = 0$  by Proposition 2.5, we get

$$\begin{aligned} (u_0 \mathcal{B}(\varepsilon) u_0^*)^D &= H + \varepsilon \frac{i}{2} (\partial_{p_k} f_\varepsilon) [u_0 (\partial_{q^k} u_0^*) - (\partial_{q^k} u_0) u_0^*]^D \\ &\quad + \varepsilon^2 \mathcal{B}_2^D + \varepsilon^{3+2\delta} \underline{R} + \varepsilon^{3+4\delta} R. \end{aligned}$$

where  $\mathcal{B}_2^D$  is made of several terms to be analyzed. We need the relations

$$\partial_{q^j} u_0^* = -u_0^* (\partial_{q^j} u_0) u_0^*, \quad (2.33)$$

$$\begin{aligned} \partial_{q^j q^{j'}}^2 u_0^* &= u_0^* (\partial_{q^{j'}} u_0) u_0^* (\partial_{q^j} u_0) u_0^* + u_0^* (\partial_{q^j} u_0) u_0^* (\partial_{q^{j'}} u_0) u_0^* - u_0^* (\partial_{q^j q^{j'}}^2 u_0) u_0^* \\ &= -(\partial_{q^{j'}} u_0^*) (\partial_{q^j} u_0) u_0^* - (\partial_{q^j} u_0^*) (\partial_{q^{j'}} u_0) u_0^* - u_0^* (\partial_{q^j q^{j'}}^2 u_0) u_0^*, \quad (2.34) \end{aligned}$$

$$\text{and} \quad [u_0 (\partial_{q^j} u_0^*)]^{OD} = -(\partial_{q^j} \Pi_0) \sigma_3, \quad (2.35)$$



coming from  $u_0^* u_0 = 1$  and the differentiation of  $u_0^* \Pi_0 u_0 = P_+$ .  
For example, the first one simplifies the  $\mathcal{O}(\varepsilon)$ -term into

$$(u_0 \mathcal{B}(\varepsilon) u_0^*)^D = H - \varepsilon i (\partial_{p_k} f_\varepsilon) [(\partial_{q^k} u_0) u_0^*]^D + \varepsilon^2 \mathcal{B}_2^D + \varepsilon^{3+2\delta} \underline{R} + \varepsilon^{3+4\delta} R.$$

Many cancellations appear after assembling all the terms in  $\mathcal{B}_2^D$ . We need accurate expressions for all of them:

- By using again  $(u_1 u_0^*)^D = 0$ , the term  $[u_0 u_2^* H + H u_2 u_0^* + u_0 u_1^* H u_1 u_0^*]^D$  equals

$$(f_\varepsilon + E_+) \Pi_0 (u_0 u_2^* + u_2 u_0^*) \Pi_0 + (f_\varepsilon + E_-) (1 - \Pi_0) (u_0 u_2^* + u_2 u_0^*) (1 - \Pi_0) \\ + (f_\varepsilon + E_-) \Pi_0 (u_0 u_1^* u_1 u_0^*) \Pi_0 + (f_\varepsilon + E_+) (1 - \Pi_0) (u_0 u_1^* u_1 u_0^*) (1 - \Pi_0).$$

In the relation

$$u_0^* u_2 + u_2^* u_0 + u_1^* u_1 + \frac{1}{2i} \{u_0^*, u_1\} + \frac{1}{2i} \{u_1^*, u_0\} = \varepsilon^{1+2\delta} \underline{R}_1 + \varepsilon^{1+4\delta} R_1,$$

the remainder terms satisfy  $R_1, \underline{R}_1 \in S_u \left( \frac{1}{\langle \sqrt{\frac{\tau'}{\tau}} q' \rangle \langle \sqrt{\tau' \tau''} p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C}) \right)$ , with the same convention as for  $R, \underline{R}$ . This identity is obtained by writing that the  $\mathcal{O}(\varepsilon^2)$  remainder of  $U^* \sharp^\varepsilon U - 1$  vanishes and by noticing that the remainder  $\underline{R}_1 + \varepsilon^{2\delta} R_1$  involves second derivatives of  $u_1$  w.r.t  $p$  and first derivatives of  $u_2$  w.r.t  $p$ . We obtain

$$[u_0 u_2^* H + H u_2 u_0^* + u_0 u_1^* H u_1 u_0^*]^D = (E_- - E_+) (u_0 u_1^* u_1 u_0^*)^D \sigma_3 \\ - \frac{1}{2i} H [u_0 \{u_0^*, u_1\} u_0^* + u_0 \{u_1^*, u_0\} u_0^*]^D + \varepsilon^{1+2\delta} \tilde{\underline{R}} + \varepsilon^{1+4\delta} \tilde{R}.$$

with  $\tilde{R}, \tilde{\underline{R}} \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , again with the same convention.

Again with  $(\partial_p u_1) u_0^* = (\partial_p u_1 u_0^*)^{OD} = \frac{(\partial_{p, p_k}^2 f)}{i(E_+ - E_-)} \partial_{q^k} \Pi_0$  and (2.35), the last factor is

$$[u_0 \{u_0^*, u_1\} u_0^* + u_0 \{u_1^*, u_0\} u_0^*]^D = -(u_0 \partial_{q^\ell} u_0^*)^{OD} \frac{(\partial_{p_\ell p_k}^2 f_\varepsilon)}{i(E_+ - E_-)} (\partial_{q^k} \Pi_0) \\ - \frac{(\partial_{p_\ell p_k}^2 f_\varepsilon)}{i(E_+ - E_-)} (\partial_{q^k} \Pi_0) ((\partial_{q^\ell} u_0) u_0^*)^{OD} \\ = -2 \frac{(\partial_{p_\ell p_k}^2 f_\varepsilon)}{i(E_+ - E_-)} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3. \quad (2.36)$$

With  $u_1 u_0^* = \frac{(\partial_{p_k} f_\varepsilon)}{i(E_+ - E_-)} (\partial_{q^k} \Pi_0)$ , we have proved

$$[u_0 u_2^* H + H u_2 u_0^* + u_0 u_1^* H u_1 u_0^*]^D = - \frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{(E_+ - E_-)} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3 \\ - H \frac{(\partial_{p_\ell p_k}^2 f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3 + \varepsilon^{1+2\delta} \tilde{\underline{R}}_1 + \varepsilon^{1+4\delta} \tilde{R}_1. \quad (2.37)$$

- The term

$$\left[ \frac{1}{2i} u_0 \{u_0^* f_\varepsilon, u_1\} u_0^* + \frac{1}{2i} u_0 \{u_1^* f_\varepsilon, u_0\} u_0^* - \frac{(\partial_{p_k} f_\varepsilon)}{2i} u_0 (\partial_{q^k} u_0^*) u_1 u_0^* \right]^D$$

equals

$$\begin{aligned} & \frac{1}{2i} f_\varepsilon [u_0 \{u_0^*, u_1\} u_0^* + u_0 \{u_1^*, u_0\} u_0^*]^D \\ & + \frac{(\partial_{p_k} f_\varepsilon)}{2i} [(\partial_{q^k} u_1) u_0^* + u_0 u_1^* (\partial_{q^k} u_0) u_0^* - u_0 (\partial_{q^k} u_0^*) u_1 u_0^*]^D. \end{aligned}$$

The diagonal part of  $(\partial_{q^k} u_1) u_0^*$  is

$$[(\partial_{q^k} u_1) u_0^*]^D = \frac{\partial_{p_\ell} f_\varepsilon}{i(E_+ - E_-)} (\partial_{q^k q^\ell}^2 \Pi_0)^D.$$

But differentiating the relation  $(\partial_{q^k} \Pi_0) \Pi_0 + \Pi_0 (\partial_{q^\ell} \Pi_0) = \partial_{q^k} \Pi_0$  w.r.t  $q^\ell$  leads to

$$(\partial_{q^k q^\ell}^2 \Pi_0)^D = -(\partial_{q^k} \Pi_0 \partial_{q^\ell} \Pi_0 + \partial_{q^\ell} \Pi_0 \partial_{q^k} \Pi_0) \sigma_3. \quad (2.38)$$

With (2.35) and  $(u_1 u_0^*) = (u_1 u_0^*)^{OD} = \frac{\partial_{p_\ell} f_\varepsilon}{i(E_+ - E_-)} \partial_{q^\ell} \Pi_0$ , we obtain

$$\begin{aligned} [u_0 u_1^* (\partial_{q^k} u_0) u_0^* - u_0 (\partial_{q^k} u_0^*) u_1 u_0^*]^D &= [-u_0 u_1^* \sigma_3 (\partial_{q^k} \Pi_0) + (\partial_{q^k} \Pi_0) \sigma_3 u_1 u_0^*] \\ &= -\frac{(\partial_{p_\ell} f_\varepsilon)}{i(E_+ - E_-)} [(\partial_{q^\ell} \Pi_0) (\partial_{q^k} \Pi_0) + (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0)] \sigma_3. \end{aligned}$$

We have found

$$\begin{aligned} & \left[ \frac{1}{2i} u_0 \{u_0^* f_\varepsilon, u_1\} u_0^* + \frac{1}{2i} u_0 \{u_1^* f_\varepsilon, u_0\} u_0^* - \frac{(\partial_{p_k} f_\varepsilon)}{2i} u_0 (\partial_{q^k} u_0^*) u_1 u_0^* \right]^D \\ &= \frac{f_\varepsilon (\partial_{p_k p_\ell}^2 f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3 + 2 \frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3. \end{aligned} \quad (2.39)$$

- The diagonal part of  $\frac{1}{2i} u_0 [\{u_0^* \mathcal{V}, u_1\} + \{u_1^* \mathcal{V}, u_0\}] u_0^*$  equals

$$\frac{1}{2i} [-u_0 (\partial_{q^k} u_0^*) \mathcal{V} (\partial_{p_k} u_1) u_0^* - (\partial_{q^k} \mathcal{V}) (\partial_{p_k} u_1) u_0^* + u_0 (\partial_{p_k} u_1^*) \mathcal{V} (\partial_{q^k} u_0) u_0^*]^D.$$

By using (2.35) with

$$\begin{aligned} (\partial_{p_k} u_1) u_0^* &= [(\partial_{p_k} u_1) u_0^*]^{OD} = \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{i(E_+ - E_-)} (\partial_{q^\ell} \Pi_0), \\ (\partial_q \mathcal{V})^{OD} &= (E_+ - E_-) (\partial_q \Pi_0), \\ \text{and} \quad E_- \Pi_0 + E_+ (1 - \Pi_0) &= \mathcal{V} + (E_- - E_+) \sigma_3, \end{aligned}$$

it becomes

$$\begin{aligned} & \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) + \frac{1}{2i} \mathcal{V} [u_0 \{u_0^*, u_1\} u_0^* + u_0 \{u_1^*, u_0\} u_0^*]^D \\ & + \frac{1}{2i} (E_- - E_+) [u_0 \{u_0^*, u_1\} u_0^* + u_0 \{u_1^*, u_0\} u_0^*]^D \sigma_3. \end{aligned}$$

The relation (2.36) yields

$$\begin{aligned} \frac{1}{2i} [u_0 \{u_0^* \mathcal{V}, u_1\} u_0^* + u_0 \{u_1^* \mathcal{V}, u_0\} u_0^*] &= -\frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \\ &+ \mathcal{V} \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{E_+ - E_-} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0). \quad (2.40) \end{aligned}$$

- The term  $\frac{1}{2i} [u_0 \{u_1^*, H\}]^D$  is the sum of two terms

$$\frac{1}{2i} [u_0 \{u_1^*, f_\varepsilon\}]^D + \frac{1}{2i} [u_0 \{u_1^*, \mathcal{V}\}]^D.$$

Since  $u_0 \partial_{p_\ell} u_1^* = i \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{(E_+ - E_-)} (\partial_{q^k} \Pi_0)$  is off-diagonal while

$$(\partial_{q^\ell} \mathcal{V})^{OD} = (E_+ - E_-) (\partial_{q^\ell} \Pi_0),$$

the second term equals

$$\frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0).$$

The first term a priori contains more terms because  $u_0^*$  has to be differentiated:

$$\begin{aligned} \frac{1}{2} \left[ -(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon) \partial_{q^\ell} \left( \frac{1}{E_+ - E_-} \right) (\partial_{q^k} \Pi_0) - \frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} (\partial_{q^\ell}^2 \Pi_0) \right. \\ \left. - u_0 (\partial_{q^\ell} u_0^*) \frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) \right]^D. \end{aligned}$$

The first part is off-diagonal and vanishes after taking the diagonal part. By using again (2.35) and (2.38) and  $\partial_q \Pi_0 = (\partial_q \Pi_0)^{OD}$ , we obtain

$$\frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3 + \frac{(\partial_{p_k} f_\varepsilon) (\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) \sigma_3 (\partial_{q^\ell} \Pi_0) = 0.$$

Hence we have proved

$$\frac{1}{2i} [u_0 \{u_1^*, H\}]^D = \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0). \quad (2.41)$$

- The last term is

$$T = \frac{1}{8} \left[ 2u_0 \{ (\partial_{p_k} f_\varepsilon)(\partial_{q^k} u_0^*), u_0 \} u_0^* \right. \\ \left. - u_0 (\partial_{q^k q^\ell}^2 u_0^*) (\partial_{p_k p_\ell}^2 f_\varepsilon) - (\partial_{p_k p_\ell}^2 f_\varepsilon) (\partial_{q^k q^\ell}^2 u_0) u_0^* \right]^D.$$

Forgetting the  $\frac{1}{8}$  factor, the first part equals  $2(\partial_{p_k p_\ell}^2 f_\varepsilon) u_0 (\partial_{q^k} u_0^*) (\partial_{q^\ell} u_0) u_0^*$ .  
By using (2.34) in the second part gives

$$8T = 4(\partial_{p_k p_\ell} f_\varepsilon) [u_0 (\partial_{q^k} u_0^*) (\partial_{q^\ell} u_0) u_0^*]^D.$$

Owing to (2.8) and (2.35), this gives

$$2T = (\partial_{p_k p_\ell}^2 f_\varepsilon) [u_0 (\partial_{q^k} u_0^*)]^D [(\partial_{q^\ell} u_0) u_0^*]^D + (\partial_{p_k p_\ell}^2 f_\varepsilon) (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0).$$

With  $u_0 (\partial_{q^k} u_0^*) = -(\partial_{q^k} u_0) u_0^*$ , the last term equals

$$T = -\frac{(\partial_{p_k p_\ell}^2 f_\varepsilon)}{2} [(\partial_{q^k} u_0) u_0^*]^D [(\partial_{q^\ell} u_0) u_0^*]^D + \frac{(\partial_{p_k p_\ell}^2 f_\varepsilon)}{2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0). \quad (2.42)$$

By summing (2.37), (2.39), (2.40), (2.41), (2.42), we obtain

$$B_2^D = -\frac{(\partial_{p_k p_\ell}^2 f_\varepsilon)}{2} [(\partial_{q^k} u_0) u_0^*]^D [(\partial_{q^\ell} u_0) u_0^*]^D + \frac{(\partial_{p_k} f_\varepsilon)(\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3 \\ + \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) + \varepsilon^{1+2\delta} \tilde{R}_1 + \varepsilon^{1+4\delta} \tilde{R}_1.$$

Hence the diagonal symbol that we seek, is

$$\begin{pmatrix} h_+ & 0 \\ 0 & h_- \end{pmatrix} = \begin{pmatrix} f_\varepsilon(p, \tau) + E_+(q, \tau) & 0 \\ 0 & f_\varepsilon(p, \tau) + E_-(q, \tau) \end{pmatrix} \\ - i\varepsilon (\partial_{p_k} f_\varepsilon) u_0^* [(\partial_{q^k} u_0) u_0^*]^D u_0 - \varepsilon^2 \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} u_0^* [(\partial_{q^k} u_0) u_0^*]^D [(\partial_{q^\ell} u_0) u_0^*]^D u_0 \\ + \varepsilon^2 \frac{(\partial_{p_k} f_\varepsilon)(\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} u_0^* (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) \sigma_3 u_0 + \varepsilon^2 \frac{\partial_{p_k p_\ell}^2 f_\varepsilon}{2} u_0^* (\partial_{q^k} \Pi_0) (\partial_{q^\ell} \Pi_0) u_0.$$

The symbol  $u_0^* [(\partial_{q^k} u_0) u_0^*]^D u_0$  equals

$$u_0^* \Pi_0 (\partial_{q^k} u_0) u_0^* \Pi_0 u_0 + u_0^* (1 - \Pi_0) (\partial_{q^k} u_0) u_0^* (1 - \Pi_0) u_0 \\ = P_+ u_0^* (\partial_{q^k} u_0) P_+ + (1 - P_+) u_0^* (\partial_{q^k} u_0) (1 - P_+) = -i \begin{pmatrix} A_k & 0 \\ 0 & -A_k \end{pmatrix}.$$

For the last term we deduce from  $\Pi_0 = u_0 P_+ u_0^*$  and  $(\partial_{q^k} u_0) u_0^* + u_0 (\partial_{q^k} u_0) = 0$ ,

$$P_+ [u_0^* (\partial_{q^k} \Pi_0) u_0] [u_0^* (\partial_{q^\ell} \Pi_0) u_0] P_+ \\ = P_+ [u_0^* (\partial_{q^k} u_0) P_+ + P_+ (\partial_{q^k} u_0^*) u_0] [u_0^* (\partial_{q^\ell} u_0) P_+ + P_+ (\partial_{q^\ell} u_0^*) u_0] P_+ \\ = P_+ u_0^* (\partial_{q^k} u_0) P_+ u_0^* (\partial_{q^\ell} u_0) P_+ + P_+ u_0^* (\partial_{q^k} u_0) P_+ (\partial_{q^\ell} u_0^*) u_0 P_+ \\ + P_+ (\partial_{q^k} u_0^*) u_0 u_0^* (\partial_{q^\ell} u_0) P_+ + P_+ (\partial_{q^k} u_0^*) u_0 P_+ (\partial_{q^\ell} u_0^*) u_0 P_+ \\ = -P_+ u_0^* (\partial_{q^k} u_0) (1 - P_+) u_0^* (\partial_{q^\ell} u_0) P_+ = X_k \overline{X}_\ell.$$

Taking the bracket with  $(1 - P_+)$  is even simpler and gives

$$\begin{aligned} (1 - P_+) [u_0^*(\partial_{q^k} \Pi_0) u_0] [u_0^*(\partial_{q^\ell} \Pi_0) u_0] (1 - P_+) \\ = -(1 - P_+) u_0^*(\partial_{q^k} u_0) P_+ u_0^*(\partial_{q^\ell} u_0) (1 - P_+) = \overline{X_k} X_\ell. \end{aligned}$$

This ends the proof.  $\square$

## 2.4 Discussion about the adiabatic approximation of the Born-Oppenheimer Hamiltonian

The Theorem 2.1 is a direct application of Proposition 2.6 by taking

$$f_\varepsilon(p) = \varepsilon^{2\delta} \tau' \tau'' |p|^2 \gamma(\tau' \tau'' |p|^2).$$

The operators

$$\begin{aligned} h_{\pm, BO}(q, \varepsilon D_q, \varepsilon) &= \varepsilon^{2\delta} \tau' \tau'' \left[ \sum_{k=1}^d (p_k \mp \varepsilon A_k)^2 \right]^{Weyl} + \varepsilon^{2+2\delta} \tau' \tau'' \sum_{k=1}^d |X_k|^2 \\ &= \varepsilon^{2+2\delta} \tau' \tau'' \left[ -\Delta + |A|^2 \mp \left[ \left( \frac{1}{i} \nabla \right) \cdot A + A \cdot \left( \frac{1}{i} \nabla \right) \right] + |X|^2 \right] \\ &= \varepsilon^{2+2\delta} \tau' \tau'' \left[ \left| \frac{1}{i} \nabla \mp A \right|^2 + |X|^2 \right], \end{aligned}$$

is nothing but the usual adiabatic effective Hamiltonians which can be found in the physics literature, including the Born-Huang potential  $|X|^2 = \sum_{k=1}^d |X_k|^2$ . We refer to [PST] and [PST2] for a discussion of the various presentations of the calculations and additional references.

Even in the region  $\left\{ \sqrt{\tau' \tau''} |p| \leq r_\gamma \right\}$  with  $p$  quantized into  $\varepsilon D_q$ , this approximation makes sense, only for  $\delta > 0$ , because of the additional term

$$\mp 2 \frac{\varepsilon^{2+4\delta} \tau' \tau''}{E_+ - E_-} \bar{X}_k X_\ell (\varepsilon \partial_{q^k}) (\varepsilon \partial_{q^\ell})$$

coming from the last terms of (2.31) and (2.32), that we have included in the remainder. It is not surprising (see [Sor], [MaSo]) that the degree of the differential operators increases with the degree in  $\varepsilon$  in the adiabatic expansion of Schrödinger type Hamiltonians. The argument of physicists says that this effective Hamiltonian is used for relatively small frequencies (or momentum) so that  $X_k X_\ell p^k p^\ell$  is negligible w.r.t  $|p - \varepsilon A|^2 + \varepsilon^2 |X|^2$ . The introduction of the additional factor  $\varepsilon^{2\delta}$  with  $\delta > 0$  provides a mathematically accurate and rather flexible implementation of this approximation.

## 3 Adaptation of the adiabatic asymptotics to the full nonlinear minimization problem

In this section, we adapt our rather general adiabatic result to our nonlinear problem. In a first step, we give an explicit form of Theorem 2.1 in our spe-

cific framework. Those results are effective when applied with wave functions localized in the frequency variable,  $\psi = \chi(\sqrt{\tau_x \tau_y} \varepsilon D_q) \psi$  for some compactly supported  $\chi$ . It could suffice if we considered minimizing the energy among such well prepared quantum states. We can do better by using a partition of unity in the frequency variable, which will be combined, in the end, with the a priori estimates coming from the complete and reduced minimization problems. Finally an estimate of the effect of the unitary transform  $\hat{U}$  on the nonlinear term is provided.

### 3.1 Adiabatic approximation for the explicit Schrödinger Hamiltonian

Let us specify the result of Theorem 2.1 by going back to the coordinates  $q = (q', q'') = (x, y)$  and  $\tau = (\tau', \tau'') = (\tau_x, \tau_y)$ . Provided that  $V_{\varepsilon, \tau}(x, y)$  fulfills the proper assumptions, the unitary transform introduced in Theorem 2.1 transforms  $H_{Lin}$  given by (1.9) into the Born-Oppenheimer Hamiltonian with a good accuracy in the low frequency region, that is when applied to wave functions  $\psi$  such that  $\psi = \chi(\sqrt{\tau_x \tau_y} \varepsilon D_q) \psi$  for some compactly supported  $\chi$ .

The operator  $H_{Lin}$  is the  $\varepsilon$ -quantization of the symbol

$$\varepsilon^{2\delta} \tau_x \tau_y |p|^2 + u_0(q, \tau) \begin{pmatrix} E_+(q, \tau, \varepsilon) & 0 \\ 0 & E_-(q, \tau, \varepsilon) \end{pmatrix} u_0(q, \tau)^*,$$

$$\text{with } E_{\pm}(q, \tau, \varepsilon) = V_{\varepsilon, \tau}(x, y) \pm \Omega \left( \sqrt{\frac{\tau_x}{\tau_y}} x \right) = V_{\varepsilon, \tau}(x, y) \pm \sqrt{1 + \frac{\tau_x}{\tau_y} x^2}.$$

The operator  $u_0(q, \tau)$  equals

$$u_0(q, \tau) = \begin{pmatrix} C & S e^{i\varphi} \\ S e^{-i\varphi} & -C \end{pmatrix} = u_0(q, \tau)^*$$

$$\text{with } C = \cos\left(\frac{\theta}{2}\right), \quad S = \sin\left(\frac{\theta}{2}\right).$$

$$\text{and } \cot(\theta) = \sqrt{\frac{\tau_x}{\tau_y}} x, \quad \varphi = \sqrt{\frac{\tau_y}{\tau_x}} y.$$

**Proposition 3.1.** *Assume  $\delta \in (0, \delta_0]$ ,  $(\tau_x, \tau_y) \in (0, 1]^2$  and assume that  $V_{\varepsilon, \tau}$  belongs to  $S_u(\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle, \frac{\frac{\tau_x}{\tau_y} dx^2}{\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle^2} + \frac{\tau_y}{\tau_x} dy^2)$  then the matricial potential*

$$\mathcal{V}(q, \tau, \varepsilon) = V_{\varepsilon, \tau}(x, y) + \Omega \left( \sqrt{\frac{\tau_x}{\tau_y}} x \right) \begin{pmatrix} \cos(\theta) & e^{i\varphi} \sin(\theta) \\ e^{-i\varphi} \sin(\theta) & -\cos(\theta) \end{pmatrix}$$

*fulfills the assumption of Theorem 2.1.*

*Choose the function  $\gamma \in \mathcal{C}_0^\infty(\mathbb{R})$  such that  $\gamma \equiv 1$  in a neighborhood of  $[-r_\gamma^2, r_\gamma^2]$ , as in Theorem 2.1 and consider a cut-off function  $\chi \in \mathcal{C}_0^\infty((-r_\gamma^2, r_\gamma^2))$ . When  $\hat{U} =$*

$U(q, \varepsilon D_q, \tau, \varepsilon) \in \text{Op}S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$  is given in Theorem 2.1, the identities

$$\begin{aligned} & \hat{U}^* H_{Lin} \hat{U} \chi(\tau_x \tau_y |\varepsilon D_q|^2) - \varepsilon^{2+4\delta} R_1(\tau, \varepsilon) = \\ & \varepsilon^{2+2\delta} \tau_x \tau_y \begin{pmatrix} e^{+i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} \hat{H}_+ e^{-i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} & 0 \\ 0 & e^{-i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} \hat{H}_- e^{i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} \end{pmatrix} \chi(\tau_x \tau_y |\varepsilon D_q|^2), \end{aligned} \quad (3.1)$$

$$\begin{aligned} & H_{Lin} \chi(\tau_x \tau_y |\varepsilon D_q|^2) - \varepsilon^{2+4\delta} R_2(\tau, \varepsilon) = \\ & \varepsilon^{2+2\delta} \tau_x \tau_y \hat{U} \begin{pmatrix} e^{+i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} \hat{H}_+ e^{-i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} & 0 \\ 0 & e^{-i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} \hat{H}_- e^{i\sqrt{\frac{\tau_y}{\tau_x}} \frac{y}{2}} \end{pmatrix} \hat{U}^* \chi(\tau_x \tau_y |\varepsilon D_q|^2), \end{aligned} \quad (3.2)$$

hold with

$$\begin{aligned} \hat{H}_+ &= -\partial_x^2 - \left( \partial_y + i \frac{x}{2\sqrt{1 + \frac{\tau_x}{\tau_y} x^2}} \right)^2 \\ &\quad + \frac{1}{\varepsilon^{2+2\delta} \tau_x \tau_y} \left[ V_{\varepsilon, \tau}(x, y) + \sqrt{1 + \frac{\tau_x}{\tau_y} x^2} \right] + W_\tau(x, y), \\ \hat{H}_- &= -\partial_x^2 - \left( \partial_y - i \frac{x}{2\sqrt{1 + \frac{\tau_x}{\tau_y} x^2}} \right)^2 \\ &\quad + \frac{1}{\varepsilon^{2+2\delta} \tau_x \tau_y} \left[ V_{\varepsilon, \tau}(x, y) - \sqrt{1 + \frac{\tau_x}{\tau_y} x^2} \right] + W_\tau(x, y), \\ W_\tau(x, y) &= \frac{\tau_x}{\tau_y(1 + \frac{\tau_x}{\tau_y} x^2)^2} + \frac{\tau_y}{\tau_x(1 + \frac{\tau_x}{\tau_y} x^2)}, \end{aligned}$$

and the estimates

$$\|R_1(\tau, \varepsilon)\|_{\mathcal{L}(L^2)} + \|R_2(\tau, \varepsilon)\|_{\mathcal{L}(L^2)} \leq C$$

which are uniform w.r.t  $\delta \in (0, \delta_0]$ ,  $\tau \in (0, 1]^2$  and  $\varepsilon \in (0, \varepsilon_0]$ .

**Proof:** Following the approach of Section 2, the Hamiltonian  $H_{Lin}$  is decomposed into

$$\begin{aligned} & H_{Lin} = H(q, \varepsilon D_q, \tau, \varepsilon) + R_\gamma(\varepsilon D_q, \tau, \varepsilon) \\ \text{with} \quad & H(q, p, \varepsilon) = \varepsilon^{2\delta} \tau_x \tau_y |p|^2 \gamma(\tau_x \tau_y |p|^2) + \left[ u_0 \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix} u_0^* \right](q, \tau), \\ \text{and} \quad & R_\gamma(p, \tau, \varepsilon) = \varepsilon^{2\delta} \tau_x \tau_y |p|^2 (1 - \gamma(\tau_x \tau_y |p|^2)). \end{aligned}$$

The Hamiltonian  $H(q, \varepsilon D_q, \tau, \varepsilon)$  fulfills the assumptions of Theorem 2.1, with the metric  $g_\tau = \frac{\frac{\tau_x}{\tau_y} dx^2}{\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle^2} + \frac{\tau_y}{\tau_x} dy^2 + \frac{\frac{\tau_x \tau_y}{\tau_x \tau_y} dp^2}{\langle \sqrt{\frac{\tau_x}{\tau_y}} p \rangle^2}$ , because we assumed

$$V_{\varepsilon, \tau} \in S_u(\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle, \frac{\frac{\tau_x}{\tau_y} dx^2}{\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle^2} + \frac{\tau_y}{\tau_x} dy^2)$$

while the gap  $E_+(q, \tau, \varepsilon) - E_-(q, \tau, \varepsilon)$  equals  $2\sqrt{1 + \frac{\tau_x}{\tau_y}x^2}$ . Actually the estimates

$$|\partial_x^\alpha \partial_y^\beta u_0(x, y)| \leq C_{\alpha, \beta} \left\langle \sqrt{\frac{\tau_x}{\tau_y}} x \right\rangle^{-|\alpha|} \left( \frac{\tau_x}{\tau_y} \right)^{\frac{|\alpha| - |\beta|}{2}}$$

are due to  $\partial_x \theta = -\frac{\sqrt{\tau_x}}{\sqrt{\tau_y}(1 + \frac{\tau_x}{\tau_y}x^2)}$  and  $\partial_y e^{i\varphi} = i\sqrt{\frac{\tau_y}{\tau_x}} e^{i\varphi}$ . Moreover the explicit computation with  $\alpha + \beta = 1$  leads to

$$\begin{pmatrix} \frac{A_x}{X_x} & X_x \\ X_x & -A_x \end{pmatrix} = iu_0^*(\partial_x u_0) = \frac{i\partial_x \theta}{2} \begin{pmatrix} 0 & e^{i\varphi} \\ -e^{-i\varphi} & 0 \end{pmatrix} \quad (3.3)$$

$$\text{and} \quad \begin{pmatrix} \frac{A_y}{X_y} & X_y \\ X_y & -A_y \end{pmatrix} = iu_0^*(\partial_y u_0) = \sqrt{\frac{\tau_y}{\tau_x}} S \begin{pmatrix} S & -Ce^{i\varphi} \\ -Ce^{-i\varphi} & -S \end{pmatrix}. \quad (3.4)$$

Hence the effective Hamiltonians  $h_{B0, \pm}(q, \varepsilon D_q, \varepsilon)$ , when restricted to the region  $\{\sqrt{\tau_x \tau_y} |p| \leq r_\gamma\}$ , are given by the symbols

$$h_{BO, \pm} = \varepsilon^{2\delta} \tau_x \tau_y \left[ p_x^2 + (p_y \mp \varepsilon \sqrt{\frac{\tau_y}{\tau_x}} \sin^2(\frac{\theta}{2}))^2 + \frac{1}{4}(|\partial_x \theta|^2 + \frac{\tau_y}{\tau_x} \sin^2(\theta)) \right] + V_{\varepsilon, \tau}(x, y) \pm \sqrt{1 + \frac{\tau_x}{\tau_y} x^2}.$$

With  $\cos(\theta) = \frac{\sqrt{\tau_x} x}{\sqrt{\tau_y} \sqrt{1 + \frac{\tau_x}{\tau_y} x^2}}$  and  $\sin(\theta) = \frac{1}{\sqrt{1 + \frac{\tau_x}{\tau_y} x^2}}$ , the Schrödinger Hamiltonian corresponding to the RHS is  $\varepsilon^{2+2\delta} \tau_x \tau_y e^{\pm i \frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}} y} \hat{H}_\pm e^{\mp i \frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}} y}$  with

$$\begin{aligned} \hat{H}_\pm = & -\partial_x^2 - \left( \partial_y \pm i \frac{x}{2\sqrt{1 + \frac{\tau_x}{\tau_y} x^2}} \right)^2 + \frac{\tau_x}{\tau_y (1 + \frac{\tau_x}{\tau_y} x^2)^2} + \frac{\tau_y}{\tau_x (1 + \frac{\tau_x}{\tau_y} x^2)} \\ & + \frac{1}{\tau_x \tau_y \varepsilon^{2+2\delta}} \left[ V_{\varepsilon, \tau}(x, y) \pm \sqrt{1 + \frac{\tau_x}{\tau_y} x^2} \right]. \end{aligned}$$

The remainder term in Theorem 2.1 is

$$\varepsilon^{2+4\delta} R_1(q, \varepsilon D_q, \tau, \varepsilon) + \varepsilon^{3+2\delta} R_2(q, \varepsilon D_q, \tau, \varepsilon),$$

with  $R_{1,2} \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$  and where  $R_2$  vanishes in a neighborhood of  $\{\sqrt{\tau_x \tau_y} |p| \leq r_\gamma\}$ . The first term provides the expected  $\mathcal{O}(\varepsilon^{2+4\delta})$  estimate in  $L^2(\mathbb{R}^2; \mathbb{C}^2)$ .

It remains to check the effect of truncations. All the factors, including the left terms

$$R_\gamma(p, \tau, \varepsilon), \quad \varepsilon^{2\delta} \tau_x \tau_y \left[ p_x^2 + (p_y \mp \varepsilon \sin^2(\frac{\theta}{2}))^2 \right] (1 - \gamma(\tau_x \tau_y |p|^2)),$$

belong to  $OpS_u(\langle \sqrt{\tau_x \tau_y} p \rangle^2, g_\tau; \mathcal{M}_2(\mathbb{C}))$ . For any  $a, b$  belonging to the class  $OpS_u(\langle \sqrt{\tau_x \tau_y} p \rangle^2, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , where  $b$  vanishes in a neighborhood of  $\{\sqrt{\tau_x \tau_y} |p| \leq r_\gamma\}$ ,



and two cut-off functions  $\chi_1, \chi_2 \in \mathcal{C}_0^\infty((-r_\gamma^2, r_\gamma^2))$  such that  $\chi_1 \prec \chi_2$  (see Definition A.3), the pseudo-differential calculus says

$$\begin{aligned} (1 - \chi_2(\tau_x \tau_y |p|^2))^\# a_\#^\varepsilon \chi_1(\tau_x \tau_y |p|^2) &\in \mathcal{N}_{u, g_\tau}, \\ b_\#^\varepsilon \chi_1(\tau_x \tau_y |p|^2) &\in \mathcal{N}_{u, g_\tau}, \end{aligned}$$

with uniform estimates of all the seminorms w.r.t  $\tau \in (0, 1]^2$  and  $\delta \in (0, \delta_0]$ . Applying this with  $\chi_1 = \chi$  and various  $\chi_2$  such that  $\chi_1 \prec \chi_2 \prec \gamma$ , implies that the remainder terms due to truncations are  $\mathcal{O}(\varepsilon^N)$  elements of  $\mathcal{L}(L^2)$  for any  $N \in \mathbb{N}$ , uniformly w.r.t  $\tau \in (0, 1]^2$  and  $\delta \in (0, \delta_0]$ . Fixing  $N \geq 2 + 4\delta_0$  ends the proof of (3.1).

For (3.2) use (3.1) with a cut-off function  $\chi_1$  such that  $\chi \prec \chi_1$  and conjugate with  $\hat{U}$  :

$$\begin{aligned} H_{Lin} \hat{U} \chi_1(\tau_x \tau_y |\varepsilon D_q|^2) \hat{U}^* &= \\ \varepsilon^{2+2\delta} \tau_x \tau_y \hat{U} \begin{pmatrix} e^{i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}} y} \hat{H}_+ e^{-i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}} y} & 0 \\ 0 & e^{-i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}} y} \hat{H}_- e^{i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}} y} \end{pmatrix} \chi_1(\tau_x \tau_y |\varepsilon D_q|^2) \hat{U}^* \\ &\quad + \varepsilon^{2+4\delta} R'_1(\varepsilon). \end{aligned}$$

Right-composing with  $\chi(\tau_x \tau_y |\varepsilon D_q|^2)$  and noticing that

$$\chi_1(\tau_x \tau_y |\varepsilon D_q|^2) \hat{U}^* \chi(\tau_x \tau_y |\varepsilon D_q|^2) - \hat{U}^* \chi(\tau_x \tau_y |\varepsilon D_q|^2) = R(q, \varepsilon D_q, \tau, \varepsilon),$$

with  $R \in \mathcal{N}_{u, g_\tau}$  lead to (3.2) like above.  $\square$

### 3.2 Linear energy estimates for non truncated states

**Proposition 3.2.** *Assume  $\delta \in (0, \delta_0]$ ,  $\tau = (\tau_x, \tau_y) \in (0, 1]^2$  and that  $V_{\varepsilon, \tau}$  belongs to the parametric symbol class  $S_u(\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle, \frac{\frac{\tau_x}{\tau_y} dx^2}{\langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle^2} + \frac{\tau_y}{\tau_x} dy^2)$ . Set  $\hat{\chi} = \chi(\tau_x \tau_y |\varepsilon D_q|^2)$  for  $\chi \in \mathcal{C}_0^\infty((-r_\gamma^2, r_\gamma^2))$ . When  $\hat{U}$  is the unitary semiclassical operator  $U(q, \varepsilon D_q, \tau, \varepsilon) \in OpS_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , given in Theorem 2.1 and parametrized by a truncation in  $\{\sqrt{\tau_x \tau_y} |p| < r_\gamma\}$ , then for any  $\chi \in \mathcal{C}_0^\infty((-r_\gamma^2, r_\gamma^2))$  the estimates*

$$\left| \left\langle \psi, [\hat{U}^* H_{Lin} \hat{U} - \varepsilon^{2+2\delta} \tau_x \tau_y H_{BO}] \psi \right\rangle \right| \leq C \varepsilon^{1+2\delta} [\varepsilon^{1+2\delta} \|\psi\|_{L^2}^2 \quad (3.5)$$

$$+ \|(1 - \hat{\chi})\psi\|_{L^2}^2 + \|(1 - \hat{\chi})\psi\|_{L^2} \times \|\sqrt{\tau_x \tau_y} |\varepsilon D_q| (1 - \hat{\chi})\psi\|_{L^2}],$$

$$\left| \left\langle \psi, [H_{Lin} - \varepsilon^{2+2\delta} \tau_x \tau_y \hat{U} H_{BO} \hat{U}^*] \psi \right\rangle \right| \leq C \varepsilon^{1+2\delta} [\varepsilon^{1+2\delta} \|\psi\|_{L^2}^2 \quad (3.6)$$

$$+ \|(1 - \hat{\chi})\psi\|_{L^2}^2 + \|(1 - \hat{\chi})\psi\|_{L^2} \times \|\sqrt{\tau_x \tau_y} |\varepsilon D_q| (1 - \hat{\chi})\psi\|_{L^2}],$$

hold uniformly w.r.t  $\tau \in (0, 1]^2$  and  $\delta \in (0, \delta_0]$ , for all  $\psi \in L^2(\mathbb{R}^2; \mathbb{C}^2)$ , with

$$\begin{aligned} H_{BO} &= \begin{pmatrix} e^{i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} \hat{H}_+ e^{-i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} & 0 \\ 0 & e^{-i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} \hat{H}_- e^{i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} \end{pmatrix} \\ \hat{H}_{\pm} &= -\partial_x^2 - \left( \partial_y \pm i \frac{x}{2\sqrt{1 + \frac{\tau_x}{\tau_y}x^2}} \right)^2 + \varepsilon^{-2-2\delta} \left[ V_{\varepsilon, \tau}(x, y) \pm \sqrt{1 + x^2} \right] \\ &\quad + W_{\tau}(x, y), \\ W_{\tau}(x, y) &= \frac{\tau_x}{\tau_y(1 + \frac{\tau_x}{\tau_y}x^2)^2} + \frac{\tau_y}{\tau_x(1 + \frac{\tau_x}{\tau_y}x^2)}. \end{aligned}$$

**Proof:** Set

$$\mathcal{D} = \hat{U}^* H_{Lin} \hat{U} - \varepsilon^{2+2\delta} \tau_x \tau_y \begin{pmatrix} e^{i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} \hat{H}_+ e^{-i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} & 0 \\ 0 & e^{-i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} \hat{H}_- e^{i\frac{\sqrt{\tau_y}}{2\sqrt{\tau_x}}y} \end{pmatrix}$$

and bound the terms  $\langle \hat{\chi} \psi, \mathcal{D} \psi \rangle$  and  $\langle (1 - \hat{\chi}) \psi, \mathcal{D} \hat{\chi} \psi \rangle$  by  $C\varepsilon^{2+4\delta} \|\psi\|_{L^2}^2$  with the help of Proposition 3.1. The remaining term is

$$\langle (1 - \hat{\chi}) \psi, \mathcal{D} (1 - \hat{\chi}) \psi \rangle, \quad \text{with} \quad \hat{\chi} = \chi(\tau_x \tau_y |\varepsilon D_q|^2).$$

The operator  $\mathcal{D}$  can be decomposed according to  $\mathcal{D} = \varepsilon^{2+2\delta} \tau_x \tau_y \mathcal{D}_{kin} + \mathcal{D}_{pot}$  with

$$\mathcal{D}_{kin} = \hat{U}^* |D_q|^2 \hat{U} - \begin{pmatrix} |D_q - A|^2 + |X|^2 & 0 \\ 0 & |D_q + A|^2 + |X|^2 \end{pmatrix}, \quad (3.7)$$

$$\mathcal{D}_{pot} = \hat{U}^* \hat{U}_0 \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix} \hat{U}_0 \hat{U} - V_{\varepsilon, \tau}(x, y) - \sqrt{1 + \frac{\tau_x}{\tau_y} x^2} \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.8)$$

The normalization in (3.8) allows to use directly the semiclassical calculus if one remembers that  $\hat{U}_0^* \hat{U} = \text{Id} + \varepsilon \hat{R}$  and  $\hat{U}^* \hat{U}_0 = \text{Id} + \varepsilon \hat{R}'$  with  $\varepsilon^{-2\delta} \hat{R}, \varepsilon^{-2\delta} \hat{R}' \in S_u(\frac{1}{\sqrt{\frac{\tau_x}{\tau_y} x}}, g_{\tau}; \mathcal{M}_2(\mathbb{C}))$  and  $E_{\pm}(q, \tau, \varepsilon) = V_{\varepsilon, \tau}(x, y) \pm \sqrt{1 + \frac{\tau_x}{\tau_y} x^2}$ . We obtain

$$|\langle (1 - \hat{\chi}) \psi, \mathcal{D}_{pot} (1 - \hat{\chi}) \psi \rangle| \leq C\varepsilon^{1+2\delta} \|(1 - \hat{\chi}) \psi\|_{L^2}^2,$$

which corresponds to the second term of our right-hand sides.

The kinetic energy term (3.7) is decomposed into

$$\varepsilon^{2+2\delta} \tau_x \tau_y \mathcal{D}_{kin} = \varepsilon^{2+2\delta} \tau_x \tau_y \mathcal{D}_{kin}^0 + \mathcal{D}_{kin}^1,$$

with

$$\mathcal{D}_{kin}^1 = \varepsilon^{2\delta} \hat{U}^* \tau_x \tau_y |\varepsilon D_q|^2 \hat{U} - \varepsilon^{2\delta} \hat{U}_0^* \tau_x \tau_y |\varepsilon D_q|^2 \hat{U}_0, \quad (3.9)$$

$$\mathcal{D}_{kin}^0 = \hat{U}_0^* |D_q|^2 \hat{U}_0 - \begin{pmatrix} |D_q - A|^2 + |X|^2 & 0 \\ 0 & |D_q + A|^2 + |X|^2 \end{pmatrix}. \quad (3.10)$$

Writing (3.9) in the form

$$\mathcal{D}_{kin}^1 = \varepsilon^{2\delta}(\hat{U}^* - \hat{U}_0^*)\tau_x\tau_y|\varepsilon D_q|^2\hat{U} + \varepsilon^{2\delta}\hat{U}_0^*\tau_x\tau_y|\varepsilon D_q|^2(\hat{U} - \hat{U}_0),$$

while  $\tau_x\tau_y|\varepsilon D_q|^2 \in OpS_u(\langle\sqrt{\tau_x\tau_y}p\rangle^2, g_\tau; \mathcal{M}_2(\mathbb{C}))$ ,  $\hat{U}, \hat{U}_0 \in OpS_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$  and  $\varepsilon^{-1-2\delta}(\hat{U} - \hat{U}_0) \in OpS_u\left(\frac{1}{\langle\sqrt{\frac{\tau_x}{\tau_y}}x\rangle\langle\sqrt{\tau_x\tau_y}p\rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ , leads to

$$|\langle(1 - \hat{\chi})\psi, \mathcal{D}_{kin}^1(1 - \hat{\chi})\psi\rangle| \leq C\varepsilon^{1+4\delta}\|(1 - \hat{\chi})\psi\|_{L^2}^2,$$

which is even smaller than the  $\mathcal{D}_{pot}$  upper bound.

In (3.10), the first term can be computed via

$$\langle\Phi, U_0^*|D_q|^2U_0(q)\Psi\rangle = \sum_{q_j \in \{x, y\}} \langle D_{q_j}(u_0(q, \tau)\Phi), D_{q_j}(u_0(q, \tau)\Psi)\rangle,$$

with  $D_{q_j}(u_0f) = u_0(D_{q_j} - iu_0^*\partial_{q_j}u_0)f$  and equals

$$\begin{aligned} \hat{U}_0^*|D_q|^2\hat{U}_0 &= |D_q - iu_0^*\partial_q u_0|^2 \\ &= \sum_{q_j \in \{x, y\}} \left[ D_{q_j}^2 - (iu_0^*(q)\partial_{q_j}u_0(q))^2 D_{q_j} - D_{q_j}(iu_0^*(q)\partial_{q_j}u_0(q))^2 \right. \\ &\quad \left. + (iu_0^*(q)\partial_{q_j}u_0(q))^2 \right]. \end{aligned}$$

Meanwhile expanding the entries of the second term in (3.10) gives

$$|D_q \mp A(q)|^2 = \sum_{q_j \in \{x, y\}} \left[ D_{q_j}^2 \mp A_j(q)D_{q_j} \mp D_{q_j}A_j(q) + A_j(q)^2 \right].$$

By using the expressions (3.3) and (3.4) for  $A, X$  and  $iu_0^*\partial_q u_0$ , we obtain

$$\begin{aligned} \mathcal{D}_{kin}^0 &= \frac{1}{2} \begin{pmatrix} 0 & R_- \\ R_+ & 0 \end{pmatrix} \\ \text{with } R_\pm &= \pm i(D_x(\partial_x\theta) + (\partial_x\theta)D_x)e^{\mp i\varphi} - \sqrt{\frac{\tau_y}{\tau_x}}\sin(\theta)(D_y e^{\mp i\varphi} + e^{\mp i\varphi}D_y) \\ \text{and } (\partial_x\theta) &= -\frac{\sqrt{\tau_x}}{\sqrt{\tau_y}(1 + \frac{\tau_x}{\tau_y}x^2)}, \quad \sin(\theta) = \frac{1}{\sqrt{1 + \frac{\tau_x}{\tau_y}x^2}}. \end{aligned}$$

Therefore, we obtain

$$|\langle(1 - \hat{\chi})\psi, \mathcal{D}_{kin}^0(1 - \hat{\chi})\psi\rangle| \leq 4 \max(\sqrt{\frac{\tau_x}{\tau_y}}, \sqrt{\frac{\tau_y}{\tau_x}}) \| |D_q|(1 - \hat{\chi})\psi \|_{L^2} \|(1 - \hat{\chi})\psi\|_{L^2}.$$

and, owing to  $\tau_x, \tau_y \in (0, 1]$ ,

$$\begin{aligned} |\langle(1 - \hat{\chi})\psi, \varepsilon^{2+2\delta}\tau_x\tau_y\mathcal{D}_{kin}^0(1 - \hat{\chi})\psi\rangle| \\ \leq 4\varepsilon^{1+2\delta}\|\sqrt{\tau_x\tau_y}|\varepsilon D_q|(1 - \hat{\chi})\psi\|_{L^2}\|(1 - \hat{\chi})\psi\|_{L^2}. \end{aligned}$$

This ends the proof of (3.5).

For (3.6) it suffices to replace  $\psi$  in (3.5) by  $\hat{U}^*\psi$  with a kinetic energy cut-off function  $\chi_1$  such that  $\chi \prec \chi_1$  and then to use  $(1 - \hat{\chi}_1)\hat{U}^*\hat{\chi} \in Op\mathcal{N}_{u,g_\tau}$ , with uniform seminorm estimates w.r.t  $\tau \in (0, 1]^2$  and  $\delta \in (0, \delta_0]$ . The  $L^2$ -norm of the corresponding additional error term is  $\mathcal{O}(\varepsilon^N)$ , for any  $N$ , and one fixes  $N \geq 2 + 4\delta_0$ .  $\square$

### 3.3 Control of the nonlinear term

In this subsection, we estimate the effect of the operator  $\hat{U} = U(q, \varepsilon D_q, \tau, \varepsilon)$  belonging to  $OpS_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$  on the nonlinear term  $\int_{\mathbb{R}^2} |\psi|^4 dx dy$ .

**Proposition 3.3.** *Let  $\hat{U}$  be the unitary operator introduced in Theorem 2.1. The inequalities*

$$\int |\psi(x, y)|^4 dx dy \geq (1 - C\varepsilon^{1+2\delta}) \int |(\hat{U}\psi)(x, y)|^4 dx dy, \quad (3.11)$$

$$\text{and} \quad \int |\psi(x, y)|^4 dx dy \geq (1 - C\varepsilon^{1+2\delta}) \int |(\hat{U}^*\psi)(x, y)|^4 dx dy \quad (3.12)$$

hold for any  $\psi \in L^4(\mathbb{R}^2; \mathbb{C}^2)$ .

**Proof:** For  $\psi_1$  and  $\psi_2$  belonging to  $L^4(\mathbb{R}^2; \mathbb{C}^2)$ , the local relations

$$\begin{aligned} |\psi_1|^4(q) &= (|\psi_2(q)|^2 + 2\operatorname{Re}\langle \psi_2(q), (\psi_1 - \psi_2)(q) \rangle + |\psi_1(q)|^2)^2 \\ &= |\psi_2(q)|^4 + 2|\psi_2|^2|\psi_1 - \psi_2|^2 + 4\left(\operatorname{Re}\langle \psi_2, \psi_1 - \psi_2 \rangle + \frac{1}{2}|\psi_1 - \psi_2|^2\right)^2 \\ &\quad + 4|\psi_2|^2\operatorname{Re}\langle \psi_2, (\psi_1 - \psi_2) \rangle \\ &\geq |\psi_2(q)|^4 - 4|\psi_2(q)|^3|\psi_1(q) - \psi_2(q)|, \end{aligned}$$

is integrated w.r.t  $q = (x, y) \in \mathbb{R}^2$ , with Hölder inequality, into

$$\|\psi_1\|_{L^4}^4 = \int |\psi_1|^4 dx dy \geq \|\psi_2\|_{L^4}^4 - 4\|\psi_2\|_{L^4}^3\|\psi_1 - \psi_2\|_{L^4}.$$

With  $\psi_1 = \hat{U}_0\psi = u_0(q)\psi$ ,  $|\psi(q)|^2 = |\psi_1(q)|^2$  for all  $q \in \mathbb{R}^2$ , and  $\psi_2 = \hat{U}\psi = \psi_1 + (\hat{U} - \hat{U}_0)\psi$ , we obtain

$$\|\psi\|_{L^4}^4 = \|\psi_1\|_{L^4}^4 \geq \|\hat{U}\psi\|_{L^4}^4 - 4\|\hat{U}\psi\|_{L^4}^3\|(\hat{U} - \hat{U}_0)\psi\|_{L^4}.$$

The operator  $\hat{U} - \hat{U}_0$  equals  $\varepsilon^{1+2\delta}r(q, \varepsilon D_q, \tau, \varepsilon)$  with  $r$  belonging to the class  $S_u\left(\frac{1}{\langle \sqrt{\frac{\tau_x}{\tau_y}}x \rangle \langle \sqrt{\tau_x \tau_y}p \rangle^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C})\right)$ , where we recall  $g_\tau = \frac{\frac{\tau_x}{\tau_y}dx^2}{\langle \sqrt{\frac{\tau_x}{\tau_y}}x \rangle^2} + \frac{\tau_y}{\tau_x}dy^2 + \frac{\tau_x \tau_y dp^2}{\langle \sqrt{\tau_x \tau_y}p \rangle^2}$ . After introducing the isometric transform on  $L^4(\mathbb{R}^2; \mathbb{C}^2)$

$$(T_{\varepsilon, \tau}\varphi)(x, y) = \varepsilon\sqrt{\tau_x \tau_y}\varphi(\varepsilon\sqrt{\tau_x \tau_y}x, \varepsilon\sqrt{\tau_x \tau_y}y),$$

the difference  $\hat{U} - \hat{U}_0$  becomes

$$\hat{U} - \hat{U}_0 = \varepsilon^{1+\delta} T_{\varepsilon, \tau}^{-1} r_1(\varepsilon \tau_x x, \varepsilon \tau_y y, D_x, D_y, \varepsilon, \tau) T_{\varepsilon, \tau}$$

with  $r_1$  uniformly bounded in  $S(1, \frac{d(\tau_x x)^2}{\langle \tau_x x \rangle^2} + d(\tau_y y)^2 + \frac{dp^2}{\langle p \rangle^2}; \mathcal{M}_2(\mathbb{C}))$ . A fortiori, the symbol  $r_1(\varepsilon \tau_x x, \varepsilon \tau_y y, \xi, \eta; \varepsilon, \tau)$  is uniformly bounded in  $S(1, dq^2 + \frac{dp^2}{\langle p \rangle^2})$  and the Lemma 3.4 below provides the uniform bound

$$\|\hat{U} - \hat{U}_0\|_{\mathcal{L}(L^4)} \leq C_0 \varepsilon^{1+\delta}.$$

We have proved

$$\|\psi\|_{L^4}^4 \geq \|\hat{U}\psi\|_{L^4}^4 - C\varepsilon^{1+2\delta} \|\hat{U}\psi\|_{L^4}^3 \|\psi\|_{L^4}.$$

which implies (3.11). The second inequality (3.12) is proved similarly with  $\hat{U}^* = \hat{U}_0^* + (\hat{U}^* - \hat{U}_0^*)$ .  $\square$

The result below is a particular case of the general  $L^p$  bound,  $1 < p < \infty$ , for pseudodifferential operator in  $OpS(1, dq^2 + \frac{dp^2}{\langle p \rangle^2}; \mathcal{L}(\mathcal{H}_1; \mathcal{H}_2))$ ,  $\mathcal{H}_i$  Hilbert spaces, stated in [Tay]-Proposition 5.7 and relying on Calderon-Zygmund analysis of singular integral operators.

**Lemma 3.4.** *For any  $p \in (1, +\infty)$ , there exists a seminorm  $\mathbf{n}$  on  $S(1, dq^2 + \frac{dp^2}{\langle p \rangle^2}; \mathcal{M}_2(\mathbb{C}))$  such that*

$$\forall a \in S(1, dq^2 + \frac{dp^2}{\langle p \rangle^2}; \mathcal{M}_2(\mathbb{C})), \quad \|a(q, D_q)\|_{\mathcal{L}(L^p)} \leq \mathbf{n}(a).$$

**Proof:** The Proposition 5.7 of [Tay] says that for any  $a \in S(1, dq^2 + \frac{dp^2}{\langle p \rangle^2}; \mathcal{M}_2(\mathbb{C}))$ , the operator  $a(q, D_q)$  is bounded on  $L^p(\mathbb{R}^2; \mathbb{C}^2)$ . It is not difficult to follow the control of the constants in the previous pages of [Tay] in order to check that  $\|a(q, D_q)\|_{\mathcal{L}(L^p)}$  is estimated by a seminorm of  $a$ . More efficiently, a linear mapping from a Fréchet space into a Banach space is continuous as soon as it is bounded on bounded sets. Apply this argument with the result of [Tay] to

$$S(1, dq^2 + \frac{dp^2}{\langle p \rangle^2}; \mathcal{M}_2(\mathbb{C})) \ni a \mapsto a(q, D_q) \in \mathcal{L}(L^p(\mathbb{R}^2; \mathbb{C}^2)).$$

$\square$

## 4 Reduced minimization problems

In this section, we assume that the potential  $V_{\varepsilon, \tau}$  satisfies (1.13)-(1.14). After the first paragraph of this section and in the rest of the paper, we focus on the case  $\tau_y = 1$ ,  $\tau_x \rightarrow 0$  (and  $\varepsilon \rightarrow 0$ ). Two reduced problems have to be considered: 1) the one obtained as  $\varepsilon \rightarrow 0$  and  $\tau_x$  is fixed; 2) the one derived from the previous

one as  $\tau_x \rightarrow 0$  and which is parametrized only by  $(G, \ell_V)$ . The linear part of this latter reduced problem is a purely quadratic Schrödinger Hamiltonian (with a constant magnetic field), from which many a priori information can be obtained. This section is divided into three parts. First we specify the potential  $V_{\varepsilon, \tau}$  and check our main assumptions for the general theory. Then we review some properties of the reduced Gross-Pitaevskii problem parametrized by  $(G, \ell_V)$ . Finally we make the comparison with the reduced Gross-Pitaevskii problem parametrized by  $(G, \ell_V, \tau_x)$  as  $\tau_x \rightarrow 0$  and deduce properties which will be necessary for the study of the complete minimization problem.

#### 4.1 Reduced minimization problems

**Lemma 4.1.** *The potential  $V_{\varepsilon, \tau}$  defined by (1.13)-(1.14) belongs to the class  $S_u \left( \langle \sqrt{\frac{\tau_x}{\tau_y}} x \rangle, g_{q, \tau} \right)$  with the metric  $g_{q, \tau} = \frac{\tau_x dx^2}{\tau_y \langle 1 + \frac{\tau_x}{\tau_y} x^2 \rangle} + \frac{\tau_y}{\tau_x} dy^2$ .*

**Proof:** After the change of variable  $(x', y') = (\sqrt{\frac{\tau_x}{\tau_y}} x, \sqrt{\frac{\tau_y}{\tau_x}} y)$ , it is equivalent to check

$$\frac{\varepsilon^{2+2\delta}}{\ell_V^2} v(\tau_y x, \tau_x y) + \sqrt{1+x^2} \varepsilon^{2+2\delta} \left[ \frac{\tau_x^2}{(1+x^2)^2} + \frac{\tau_y^2}{1+x^2} \right] \in S_u(\langle x \rangle, \frac{dx^2}{\langle x \rangle^2} + dy^2).$$

It is done if  $v(\tau_y x, \tau_x y) \in S_u(\langle x \rangle, \frac{dx^2}{\langle x \rangle^2} + dy^2)$ . We know  $v \in S(1, \frac{dx^2+dy^2}{1+x^2+y^2})$ . Hence for all  $(\alpha, \beta) \in \mathbb{N}^2$  there exists  $C_{\alpha, \beta} > 0$  such that

$$\begin{aligned} \forall \tau \in (0, 1]^2, \forall x, y \in \mathbb{R}^2, \quad |\partial_x^\alpha \partial_y^\beta (v(\tau_y x, \tau_x y))| &\leq C_{\alpha, \beta} \frac{\tau_x^\beta \tau_y^\alpha}{(1 + \tau_y^2 x^2 + \tau_x^2 y^2)^{-\frac{\alpha+\beta}{2}}} \\ &\leq C_{\alpha, \beta} \frac{1}{(\frac{1}{\tau_y^2} + x^2)^{\alpha/2}} \leq C_{\alpha, \beta} \langle x \rangle^{1-|\alpha|}, \end{aligned}$$

which is what we seek.  $\square$

If the error terms of Proposition 3.2 and Proposition 3.3 are assumed to be negligible, the energy  $\mathcal{E}_\varepsilon(\psi)$  of a state  $\psi = \hat{U}^* \begin{pmatrix} 0 \\ a_- \end{pmatrix}$  is close to

$$\begin{aligned} \varepsilon^{2+2\delta} \tau_x \tau_y \langle a_-, \hat{H}_- a_- \rangle + \frac{G_{\varepsilon, \tau}}{2} \int |a_-|^4 dx dy &= \varepsilon^{2+2\delta} \tau_x \tau_y \mathcal{E}_\tau(a_-), \\ \text{with } \mathcal{E}_\tau(a_-) &= \langle a_-, \hat{H}_- a_- \rangle + \frac{G}{2} \int |a_-|^4 dx dy, \\ \hat{H}_- &= -\partial_x^2 - \left( \partial_y - i \frac{x}{2\sqrt{1 + \frac{\tau_x}{\tau_y} x^2}} \right)^2 + \frac{1}{\ell_V^2 \tau_x \tau_y} v(\sqrt{\tau_x \tau_y} x, \sqrt{\tau_x \tau_y} y). \end{aligned} \tag{4.1}$$

with the potential  $v$  chosen from (1.14).

When  $\frac{\tau_x}{\tau_y}$  and  $\tau_x \tau_y$  are small, in particular in the regime  $\tau_x \ll 1$  and  $\tau_y = 1$  that

we shall consider, this energy is well approximated by

$$\mathcal{E}_H(\varphi) = \langle \varphi, \left[ -\partial_x^2 - (\partial_y - \frac{ix}{2})^2 + \frac{x^2 + y^2}{\ell_V^2} \right] \varphi \rangle + \frac{G}{2} \int |\varphi|^4, \quad (4.2)$$

as this will be checked and specified in the next paragraph. Although more general asymptotics could be considered, we concentrate from now on the regime  $\tau_x \ll 1$ ,  $\tau_y = 1$ . The parameters  $\ell_V$  and  $G$  are assumed to be fixed as  $\tau_x \rightarrow 0$ .

In order to prove that the ground states of  $\mathcal{E}_H$  and  $\mathcal{E}_\varepsilon$  are close, we need good estimates on the energy  $\mathcal{E}_H$ .

## 4.2 Properties of the harmonic approximation

The energy functional  $\mathcal{E}_H$  does not any more depend on  $\tau_x$  and is parametrized only by  $(G, \ell_V)$ . Let us start with its properties. We introduce the spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  which are given by

$$\mathcal{H}_s = \left\{ u \in L^2(\mathbb{R}^2) \mid \sum_{|\alpha|+|\beta| \leq s} \|q^\alpha D_q^\beta u\|_{L^2} < +\infty \right\}, \quad s = 1, 2, (q = (x, y)) \quad (4.3)$$

endowed with the norm  $\|u\|_{\mathcal{H}_s}^2 = \sum_{|\alpha|+|\beta| \leq s} \|q^\alpha D_q^\beta u\|_{L^2}^2$ . For a compact set  $K$  of  $\mathcal{H}_s$  and for  $u \in \mathcal{H}_s$ , the distance  $d_s(u, K)$  follows the usual definition  $\min_{v \in K} \|u - v\|_{\mathcal{H}_s}$ . The self-adjoint operator associated with the linear part of  $\mathcal{E}_H$  is denoted by

$$H_{\ell_V} = -\partial_x^2 - (\partial_y - \frac{ix}{2})^2 + \frac{x^2 + y^2}{\ell_V^2}, \quad (0 < \ell_V < +\infty).$$

Its domain is  $\mathcal{H}_2$  while its form domain is  $\mathcal{H}_1$ . Note also the compact embeddings  $\mathcal{H}_2 \subset \subset \mathcal{H}_1 \subset \subset L^2 \cap L^4$ . Following the general scheme presented in [HiPr, Sjo], its spectrum equals

$$\sigma(H_{\ell_V}) = \{(1 + 2n_+)r_+ + (1 + 2n_-)r_-, \quad (n_+, n_-) \in \mathbb{N}^2\}$$

$$\text{with } r_\pm = \frac{1}{2\sqrt{2}} \sqrt{1 + \frac{8}{\ell_V^2} \pm \sqrt{1 + \frac{4}{\ell_V^2}}}.$$

**Proposition 4.2.** *The functional  $\mathcal{E}_H$  admits minima on  $\{u \in \mathcal{H}_1, \|u\|_{L^2} = 1\}$ , with a minimum value  $\mathcal{E}_{H,min}$  satisfying*

$$\mathcal{E}_{H,min} \geq r_+ + r_- \geq \frac{\sqrt{2}}{2}.$$

*The set of minimizers  $\text{Argmin } \mathcal{E}_H$  is a bounded subset of  $\mathcal{H}_2$  and therefore a compact subset of  $\{u \in \mathcal{H}_1, \|u\|_{L^2} = 1\}$ . Moreover for any  $\varphi \in \text{Argmin } \mathcal{E}_H$ ,  $\varphi$  is an eigenvector of  $H_0 + G|\varphi|^2$ . Finally there exist two constants  $C = C_{\ell_V, G} > 0$  and  $\nu = \nu_{\ell_V, G} \in (0, 1/2]$  such that the conditions  $u \in \mathcal{H}_1$ ,  $\|u\|_{L^2} = 1$  and  $\mathcal{E}_H(u) \leq \mathcal{E}_{H,min} + 1$ , imply*

$$d_{\mathcal{H}_1}(u, \text{Argmin } \mathcal{E}_H) \leq C(\mathcal{E}_H(u) - \mathcal{E}_{H,min})^\nu. \quad (4.4)$$

**Proof:** On  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , the scalar products

$$\begin{aligned}\langle u, v \rangle_{1, \ell_V} &= \langle u, H_{\ell_V} v \rangle_{L^2} \\ \langle u, v \rangle_{2, \ell_V} &= \langle H_{\ell_V} u, H_{\ell_V} v \rangle_{L^2}\end{aligned}$$

provide norms  $\|u\|_{k, \ell_V}$ ,  $k = 1, 2$ , respectively equivalent to  $\|u\|_{\mathcal{H}_k}$ . In this proof, all the “uniform” estimates are actually parametrized by  $(G, \ell_V)$ . The nonlinearity  $\frac{G}{2} \int |u|^4(x) dx$  as well as the constraint  $\|u\|_{L^2} = 1$  are continuous functions on  $L^2 \cap L^4$  while the quadratic part of  $\mathcal{E}_H(u)$  is simply  $\|u\|_{1, \ell_V}^2$  with  $\mathcal{E}_H(u) \geq \|u\|_{1, \ell_V}^2 \geq r_+ + r_- \geq \frac{\sqrt{2}}{2}$ . The compact embedding  $\mathcal{H}_1 \subset\subset L^2 \cap L^4$  thus implies that the infimum  $\inf_{u \in \mathcal{H}_1, \|u\|_{L^2}=1} \mathcal{E}_H(u)$  is achieved. A minimizer  $\varphi \in \text{Argmin } \mathcal{E}_H$  solves in a distributional sense the Euler-Lagrange equation

$$H_{\ell_V} \varphi + G|\varphi|^2 u = \lambda_\varphi \varphi$$

where  $\lambda_\varphi$  is the Lagrange multiplier associated with the constraint  $\|\varphi\|_{L^2} = 1$ . By taking the scalar product with  $\varphi$ , one obtains the bounds for  $\lambda_\varphi$ :

$$\mathcal{E}_{H, \min} \leq \lambda_\varphi \leq 2\mathcal{E}_{H, \min}.$$

Since  $\mathcal{H}_1$  is also (compactly) embedded in  $L^6(\mathbb{R}^2)$ , the equation

$$H_{\ell_V} \varphi = -G|\varphi|^2 \varphi + \lambda_\varphi \varphi$$

ensures that  $\|\varphi\|_{2, \ell_V}$  is uniformly bounded on  $\text{Argmin } \mathcal{E}_H$ . Therefore  $\text{Argmin } \mathcal{E}_H$  is a bounded subset of  $\mathcal{H}_2$  and a compact subset of  $\mathcal{H}_1$ . In an  $\mathcal{H}_1$ -neighborhood of  $\varphi \in \text{Argmin } \mathcal{E}_H$  ( $\|\varphi\|_{L^2} = 1$ ), the  $L^2$ -sphere  $\{u \in \mathcal{H}_1, \|u\|_{L^2} = 1\}$  can be parametrized by

$$u = (1 - \|v\|_{L^2}^2)\varphi + v, \quad \langle \varphi, v \rangle_{L^2} = 0.$$

Notice also that the potential  $G|\varphi|^2$  is a relatively compact perturbation of  $H_{\ell_V}$ , so that  $H_{\ell_V} + G|\varphi|^2$  is a self-adjoint operator in  $L^2(\mathbb{R}^2)$  with domain  $\mathcal{H}_2$  and with a compact resolvent. With  $\langle \varphi, v \rangle_{1, \ell_V} = -G \int_{\mathbb{R}^2} |\varphi|^2 \bar{\varphi} v dx$  for  $\varphi$  is an eigenvector of  $H_{\ell_V} + G|\varphi|^2$  and  $v \perp \varphi$ , the energy  $\mathcal{E}_H(u)$  becomes

$$\begin{aligned}\mathcal{E}_H((1 - \|v\|_{L^2}^2)\varphi + v) &= \|v\|_{1, \ell_V}^2 + (1 - \|v\|_{L^2}^2) \langle \varphi, \varphi \rangle_{1, \ell_V} \\ &\quad - 2G(1 - \|v\|_{L^2}^2) \text{Re} \int_{\mathbb{R}^2} |\varphi|^2 \bar{\varphi} v dx + \frac{G}{2} \int_{\mathbb{R}^2} |(1 - \|v\|_{L^2}^2)\varphi + v|^4 dx \\ &= \|v\|_{1, \ell_V}^2 + F_\varphi(v),\end{aligned}$$

where  $v$  lies in the closed subset  $\mathcal{H}_{1, \varphi} = \{v \in \mathcal{H}_1, \langle \varphi, v \rangle_{L^2} = 0\}$  of  $\mathcal{H}_1$  and  $F_\varphi(v)$  is the composition of the compact embedding  $\mathcal{H}_1 \rightarrow L^2 \cap L^4$  with a real analytic, real-valued, functional on  $L^2 \cap L^4$ . Hence on  $\mathcal{H}_{1, \varphi}$  endowed with the scalar product  $\langle \cdot, \cdot \rangle_{1, \ell_V}$ , the Hessian of  $\mathcal{E}_H((1 - \|v\|_{L^2}^2)\varphi + v)$  equals  $\text{Id} + D^2 F_{\ell_V}(0)$ , with  $D^2 F_{\ell_V}(0)$  compact (and self-adjoint). We can apply the Lojasiewicz-Simon inequality which says that there exist two constants  $C_\varphi > 0$ ,  $\nu_\varphi \in (0, 1/2]$ , such that

$$\|v\|_{1, \ell_V} \leq C_\varphi (\mathcal{E}_H((1 - \|v\|_{L^2}^2)\varphi + v) - \mathcal{E}_{H, \min})^{\nu_\varphi}.$$



Since the set  $\text{Argmin } \mathcal{E}_H$  is a compact subset of  $\mathcal{H}_1$ , it can be covered by a finite number of neighborhoods of  $\varphi_i \in \text{Argmin } \mathcal{E}_H$ ,  $1 \leq i \leq N$ , where a Lojasiewicz-Simon inequality holds. Take

$$\nu_{\ell_V, G} = \min_{1 \leq i \leq N} \nu_{\varphi_i} \quad \text{and} \quad C_{\ell_V, G} = 2 \max_{1 \leq i \leq N} C_{\varphi_i}.$$

□

**Remark 4.3.** *The Lojasiewicz inequality is a classical result of real algebraic geometry (see a.e. [Loj, BCR]) proved by Lojasiewicz after Tarski-Seidenberg Theorem. It is usually written as  $|\nabla f(x)| \leq C|f(x)|^\nu$  with  $\nu \in (0, 1]$  for a real analytic function of  $x$  lying around  $x_0$  with  $f(x_0) = 0$ . The variational form is a variant of it. It was extended to the infinite dimensional case with applications to PDE's by L. Simon in [Sim]. We refer the reader also to [Chi, HaJe, Hua] and [BDLM] for recent texts and references concerned with the infinite dimensional case or the extension with o-minimal structures.*

*The nonlinear Euler-Lagrange equation is usually studied after linearization via the Liapunov-Schmidt process. Here using some coordinate representation of the constraint submanifold, especially when it is a sphere for a simple norm, allows to use directly the standard result for the minimization of real analytic functionals.*

*When the minimization problem is non degenerate at every  $\varphi \in \text{Argmin } \mathcal{E}_H$ , i.e. in the present case when the kernel of  $\text{Id} + D^2 F_\varphi(0)$  is restricted to  $\{0\}$ , the compact set  $\text{Argmin } \mathcal{E}_H$  is made of a finite number of point. When  $\ell_V$  is fixed so that  $r_+$  and  $r_-$  are rationally independent, the spectrum of  $H_{\ell_V}$  is made of simple eigenvalues and when  $G$  is small enough,  $G < G_{\ell_V}$ , the non degeneracy assumption is satisfied via a perturbation argument from the case  $G = 0$ . For large  $G$ , we can only say that the set of  $(G, \ell_V) \in (0, +\infty)^2$  such that all the minima are non degenerate,  $\nu_{\ell_V, G} = 1/2$ , is a subanalytic subset of  $\mathbb{R}^2$ . In our case with a linear part  $H_{\ell_V}$  which is a complex operator with no rotational symmetry, no standard methods like in [AJR] allow to reduce the minimization problem to some radial nonlinear ODE.*

*From the information given by the Lowest-Landau-Level reduction, when  $G$  and  $\ell_V$  are large, the supposed hexagonal symmetry, after removing some trivial rotational invariance, of the problem (see [ABN, Nie]) suggests that there are presumably several minimizers.*

A change of variable  $\varphi(x, y)e^{-ixy/4} = \alpha u(\alpha x, \alpha y)$  with  $\alpha^2 = 1/(\ell_V \sqrt{G})$  leads to

$$\mathcal{E}_H(\varphi) = \frac{1}{\ell_V \sqrt{G}} \tilde{\mathcal{E}}_H(u) = \frac{1}{\ell_V \sqrt{G}} \int |(\nabla - \frac{i}{2} \ell_V \sqrt{G} e_z \times \vec{r})u|^2 + G(r^2 |u|^2 + \frac{1}{2} |u|^4), \quad (4.5)$$

with the notations  $\vec{r} = \begin{pmatrix} x \\ y \end{pmatrix}$   $r = |\vec{r}|$ . This implies that  $\ell_V \sqrt{G}$  is equivalent to a rotation value. We have the following results from the literature

- when  $\ell_V \sqrt{G}$  is small and  $G$  is large, the minimizer is unique up to rotation and vortex-free [AJR]: namely  $u(x, y) = f(r)e^{ic}$  for some real number  $c$ , where  $f$  does not vanish. If  $\ell_V \sqrt{G} = 0$ , this is an adaptation of a result of [BrOs]. When  $\ell_V \sqrt{G}$  is non zero, this requires refined estimates for the jacobian.
- when  $\ell_V \sqrt{G}$  is large, then vortices are expected in the system and this can be analyzed in details in the LLL regime (lowest Landau level) if additionally  $\sqrt{G}/\ell_V$  is small [AB, ABN]. More precisely, if  $\sqrt{G}/\ell_V$  is small, then

$$\inf \tilde{\mathcal{E}}_H - \frac{1}{2} - \inf E_{LLL} = o\left(\frac{\sqrt{G}}{\ell_V}\right) \quad (4.6)$$

where

$$E_{LLL}(u) = \int G(r^2|u|^2 + \frac{1}{2}|u|^4) \quad (4.7)$$

for functions  $u$  such that  $u(x, y)e^{\ell_V \sqrt{G} r^2/4}$  is a holomorphic function of  $x + iy$ . This space is called the LLL. If  $u$  is a ground state of  $\tilde{\mathcal{E}}_H$  and  $w$  its projection onto the LLL, then  $|u - w|$  tends to 0 in  $H^1$  and  $C^{0,\alpha}$  as  $\sqrt{G}/\ell_V$  tends to 0. If additionally,  $\ell_V \sqrt{G}$  is large, then one can estimate  $\inf E_{LLL}$  [ABN] thanks to test functions with vortices and  $\inf E_{LLL} = O\left(\frac{\sqrt{G}}{\ell_V}\right)$ .

- if  $\ell_V \sqrt{G}$  is large, and  $\sqrt{G}/\ell_V$  is large, then this is a Thomas Fermi regime where the energy can be estimated as well [Aft] and is of order  $\sqrt{G}/\ell_V$ .

We complete the previous result with another comparison statement which will be useful in the sequel.

**Proposition 4.4.** *There exists  $C = C_{\ell_V, G} > 0$  such that when  $u \in \mathcal{H}_1$  satisfy  $\mathcal{E}_H(u) \leq \mathcal{E}_{H, \min} + 1$ ,  $\|u\|_{L^2} = 1$ , and solves*

$$H_{\ell_V, G} u + G|u|^2 u = \lambda_u u + r$$

with  $\lambda_u \in \mathbb{R}$  and  $r \in L^2$ , then

- $u \in \mathcal{H}_2$ ;
- there exists  $u_0 \in \text{Argmin } \mathcal{E}_H$ , with Lagrange multiplier  $\lambda_{u_0}$ , such that

$$|\lambda_u - \lambda_{u_0}| + \|u - u_0\|_{\mathcal{H}_2} \leq C(\|r\|_{L^2} + (\mathcal{E}_H(u) - \mathcal{E}_{H, \min})^\nu),$$

where  $\nu = \nu_{\ell_V, G} \in (0, \frac{1}{2}]$  is the exponent given in Proposition 4.2.

**Proof:** Since  $\text{Argmin } \mathcal{E}_H$  is compact, Proposition 4.2 already provides  $u_0 \in \text{Argmin } \mathcal{E}_H$  such that

$$\|u - u_0\|_{\mathcal{H}_1} \leq C(\mathcal{E}_H(u) - \mathcal{E}_{H, \min})^\nu.$$

Taking the difference of the equation for  $u$  and the Euler-Lagrange equation for  $u_0$ , we obtain

$$H_{\ell_V, G}(u - u_0) = (\lambda_u - \lambda_{u_0})u_0 + \lambda_u(u - u_0) + G(|u_0|^2 u_0 - |u|^2 u) + r.$$

Taking the scalar product with  $u_0$ , with

$$\| |u_0|^2 u_0 - |u|^2 u \|_{L^2} \leq C (\mathcal{E}_H(u_0) + \mathcal{E}_H(u)) \|u - u_0\|_{\mathcal{H}_1} \leq C' (\mathcal{E}_H(u) - \mathcal{E}_{H, \min})^\nu$$

implies

$$|\lambda_u - \lambda_{u_0}| \leq C'' (\|r\|_{L^2} + (\mathcal{E}_H(u) - \mathcal{E}_{H, \min})^\nu).$$

Using the ellipticity of  $H_{\ell_V, G}$  and the equivalence of the norms  $\|\varphi\|_{\mathcal{H}_2}$  and  $\|H_{\ell_V, G}\varphi\|_{L^2}$  ends the proof.  $\square$

### 4.3 Comparison of the two reduced minimization problems

In the regime  $\tau_y = 1$  and  $\tau_x \rightarrow 0$ , while  $\ell_V > 0$  and  $G > 0$  are fixed, we compare the two minimization problems for the energies  $\mathcal{E}_\tau$  and  $\mathcal{E}_H$  defined in (4.1)-(4.2). We start with the next Lemma which is a simple application of the so called IMS localization formula (see a.e. [CFKS]). We shall use the functional spaces  $\mathcal{H}_s$  defined by (4.3) associated with  $\mathcal{E}_H$  as well as the standard Sobolev spaces  $H^s(\mathbb{R}^2)$  associated with  $\mathcal{E}_\tau$ , with  $s = 1, 2$  and  $\mathcal{H}_s \subset H^s(\mathbb{R}^2)$ .

**Lemma 4.5.** *Let  $\chi_1, \chi_2 \in \mathcal{C}_b^\infty(\mathbb{R}^2)$  satisfy  $\chi_1^2 + \chi_2^2 = 1$ ,  $\text{supp } \chi_1 \subset \{x^2 + y^2 < 1\}$  and take  $\alpha \in (0, \frac{1}{2}]$ . Then the following identity*

$$\begin{aligned} \mathcal{E}_H(u) &= \mathcal{E}_H(\chi_1(\tau_x^\alpha \cdot)u) + \mathcal{E}_H(\chi_2(\tau_x^\alpha \cdot)u) - \tau_x^{2\alpha} \sum_{j=1}^2 \int_{\mathbb{R}^2} |(\nabla \chi_j)(\tau_x^\alpha \cdot)|^2 |u|^2 \\ &\quad + G \int_{\mathbb{R}^2} (\chi_1^2 \chi_2^2)(\tau_x^\alpha \cdot) |u|^4, \end{aligned} \quad (4.8)$$

holds for all  $u \in \mathcal{H}_1$ , with the same formula for  $\mathcal{E}_\tau(u)$  when  $u \in H^1(\mathbb{R}^2)$ . Moreover,  $\mathcal{E}_\tau$  and  $\mathcal{E}_H$  satisfy

$$\begin{aligned} \mathcal{E}_\tau(u) &= \mathcal{E}_H(\chi_1(\tau_x^\alpha \cdot)u) + \mathcal{E}_\tau(\chi_2(\tau_x^\alpha \cdot)u) - \tau_x^{2\alpha} \sum_{j=1}^2 \int_{\mathbb{R}^2} |(\nabla \chi_j)(\tau_x^\alpha \cdot)|^2 |u|^2 \\ &\quad + G \int_{\mathbb{R}^2} (\chi_1^2 \chi_2^2)(\tau_x^\alpha \cdot) |u|^4 + R(u), \end{aligned} \quad (4.9)$$

for all  $u \in H^1(\mathbb{R}^2)$  with

$$|R(u)| \leq \frac{1}{4} \left( \mathcal{E}_\tau(\chi_1(\tau_x^\alpha \cdot)u)^{1/2} + \mathcal{E}_H(\chi_1(\tau_x^\alpha \cdot)u)^{1/2} \right) \|u\|_{L^2 \tau_x^1}^{1-3\alpha}.$$

**Proof:** The first identity is a direct application of the IMS localization formula (see a.e. [CFKS]) which comes from the identity

$$P\chi^2P - \chi P^2\chi = [P, \chi]^2 - \frac{1}{2} [\chi^2, P] P - \frac{1}{2} P [P, \chi^2]$$

when  $P$  is a differential operator of order  $\leq 1$  and  $\chi$  is a  $C^\infty$  function. Simply combine it with the identity

$$|u|^4 = |\chi_1(\tau_x^\alpha \cdot)u|^4 + |\chi_2(\tau_x^\alpha \cdot)u|^4 + 2\chi_1^2\chi_2^2(\tau_x^\alpha \cdot)|u|^4.$$

Using the same argument for  $\mathcal{E}_\tau$  provides the same identity after replacing  $\mathcal{E}_H$  with  $\mathcal{E}_\tau$ , and it suffices to compare  $\mathcal{E}_\tau(\chi_1(\tau_x^\alpha \cdot)u)$  with  $\mathcal{E}_H(\chi_1(\tau_x^\alpha \cdot)u)$ . The definition (1.14) of the potential  $v$  and the condition  $\alpha \leq \frac{1}{2}$  imply

$$v(\tau_x^{1/2} \cdot) = \tau_x(x^2 + y^2) \quad \text{on } \text{supp } \chi_1(\tau_x^\alpha \cdot).$$

Therefore, we obtain, by setting  $u_\tau = \chi_1(\tau_x^\alpha \cdot)u$ ,

$$\begin{aligned} & |\mathcal{E}_\tau(\chi_1(\tau_x^\alpha \cdot)u) - \mathcal{E}_H(\chi_1(\tau_x^\alpha \cdot)u)| = \\ & \left| \int_{\mathbb{R}^2} |(\partial_y - i \frac{x}{2\sqrt{1+\tau_x x^2}})u_\tau|^2 - |(\partial_y - i \frac{x}{2})u_\tau|^2 \right| \\ & \leq \left( \|(\partial_y - i \frac{x}{2\sqrt{1+\tau_x x^2}})u_\tau\|_{L^2} + \|(\partial_y - i \frac{x}{2})u_\tau\|_{L^2} \right) \\ & \quad \times \left\| \frac{\tau_x x^3/2}{1 + \sqrt{1 + \tau_x x^2}} \chi_1(\tau_x^\alpha \cdot)u \right\|_{L^2} \\ & \leq \frac{1}{4} \left( \mathcal{E}_\tau(\chi_1(\tau_x^\alpha \cdot)u)^{1/2} + \mathcal{E}_H(\chi_1(\tau_x^\alpha \cdot)u)^{1/2} \right) \|u\|_{L^2} \tau_x^{1-3\alpha}. \end{aligned}$$

□

**Proposition 4.6.** *For any given  $(\ell_V, G) \in (0, +\infty)^2$ , there exists  $\tau_{\ell_V, G} > 0$  such that the following properties hold when  $\tau_x \leq \tau_{\ell_V, G}$ .*

- *The minimization problem*

$$\inf_{u \in H^1(\mathbb{R}^2), \|u\|_{L^2}=1} \mathcal{E}_\tau(u)$$

*admits a solution  $u \in H^1(\mathbb{R}^2)$ .*

- *A solution  $u \in H^1(\mathbb{R}^2)$  to the above minimization problem, solves an Euler-Lagrange equation*

$$\left[ -\partial_x^2 - (\partial_y - i \frac{x}{2\sqrt{1+\tau_x x^2}})^2 + \frac{v(\tau_x^{1/2} \cdot)}{\ell_V^2 \tau_x} + G|u|^2 \right] u = \lambda_u u$$

*with  $0 \leq \lambda_u \leq 2\mathcal{E}_{\tau, \min}$  and belongs to  $H^2(\mathbb{R}^2)$ .*

- Moreover the minimum value  $\mathcal{E}_{\tau, \min} = \min_{u \in H^1(\mathbb{R}^2), \|u\|_{L^2}=1} \mathcal{E}_{\tau}(u)$  satisfies the estimate

$$|\mathcal{E}_{\tau, \min} - \mathcal{E}_{H, \min}| \leq C_{\ell_V, G} \tau_x^{2/3}.$$

- For  $u \in \text{Argmin } \mathcal{E}_{\tau}$  and any pairs  $\chi = (\chi_1, \chi_2)$  in  $\mathcal{C}_b^{\infty}(\mathbb{R}^2)^2$  such that  $\chi_1^2 + \chi_2^2 = 1$  with  $\text{supp } \chi_1 \subset \{x^2 + y^2 < 1\}$  and  $\chi_1 \equiv 1$  in  $\{x^2 + y^2 \leq 1/2\}$ , the functions  $\chi_j(\tau_x^{1/9} \cdot)u$ ,  $j = 1, 2$ , satisfy

$$\|\chi_2(\tau_x^{1/9} \cdot)u\|_{L^2}^2 \leq C_{\chi, \ell_V, G} \tau_x^{2/3} \quad (4.10)$$

$$\mathcal{E}_{\tau}(\chi_1(\tau_x^{1/9} \cdot)u) \leq \mathcal{E}_{\tau, \min} + C_{\chi, \ell_V, G} \tau_x^{2/3} \quad (4.11)$$

$$d_{\mathcal{H}_2}(\chi_1(\tau_x^{1/9} \cdot)u, \text{Argmin } \mathcal{E}_H) \leq C_{\chi, \ell_V, G} \tau_x^{2\nu_{\ell_V, G}/3}, \quad (4.12)$$

$$\nu_{\ell_V, G} \in (0, \frac{1}{2}]. \quad (4.13)$$

A constant  $C_{a,b,c}$  is a constant which is fixed once  $(a, b, c)$  are given.

**Proof:** Fix  $\ell_V$  and  $G$ . We drop the indices  $\ell_V, G$  in the constants. The exponent  $\alpha$  will be fixed to the value  $\frac{1}{9}$  within the proof.

First step, upper bound for  $\inf\{\mathcal{E}_{\tau}(u), u \in H^1(\mathbb{R}^2), \|u\|_{L^2} = 1\}$ :

Let  $\chi = (\chi_1, \chi_2)$  and  $\tilde{\chi} = (\tilde{\chi}_1, \tilde{\chi}_2)$  be two pairs as in our statement such that  $\tilde{\chi}_1 \prec \chi_1$  according to Definition A.3. Take  $u_0 \in \text{Argmin } \mathcal{E}_H \subset \mathcal{H}_1$ . According to Proposition 4.2, it belongs to a bounded set of  $\mathcal{H}_2$  so that  $\| |q|^2 u_0 \|_{L^2}$ , with  $q = (x, y)$ , is uniformly bounded. Hence,  $0 \notin \text{supp } \nabla \tilde{\chi}_j \cup \text{supp } \tilde{\chi}_1 \tilde{\chi}_2$  implies

$$\int_{\mathbb{R}^2} |\nabla \tilde{\chi}_j(\tau_x^{\alpha} \cdot)|^2 |u_0|^2 = \mathcal{O}(\tau_x^{4\alpha}) \quad \text{while} \quad \int_{\mathbb{R}^2} \tilde{\chi}_1^2 \tilde{\chi}_2^2(\tau_x^{\alpha} \cdot) |u_0|^4 \geq 0.$$

Lemma 4.5 above with the pair  $\tilde{\chi}$  and  $\alpha \in (0, \frac{1}{2}]$  gives:

$$\mathcal{E}_{H, \min} = \mathcal{E}_H(u_0) \geq \mathcal{E}_H(\tilde{\chi}_1(\tau_x^{\alpha} \cdot)u_0) + \mathcal{E}_H(\tilde{\chi}_2(\tau_x^{\alpha} \cdot)u_0) - C\tau_x^{6\alpha}.$$

On  $\text{supp } \tilde{\chi}_2(\tau_x^{\alpha} \cdot)$ , the potential  $\frac{v(\tau_x^{1/2} \cdot)}{\ell_V^2 \tau_x}$  is bounded from below by  $\frac{1}{C'\tau_x^{2\alpha}}$ . Thus we get

$$\mathcal{E}_{H, \min} (\|\tilde{\chi}_1 u_0\|_{L^2}^2 + \|\tilde{\chi}_2 u_0\|_{L^2}^2) \geq \mathcal{E}_{H, \min} \|\tilde{\chi}_1 u_0\|_{L^2}^2 + \frac{1}{C'\tau_x^{2\alpha}} \|\tilde{\chi}_2 u_0\|_{L^2}^2 - C\tau_x^{6\alpha},$$

and finally

$$\|\tilde{\chi}_2 u_0\|_{L^2}^2 \leq C'' \tau_x^{8\alpha}, \quad \|\tilde{\chi}_1 u_0\|_{L^2}^2 = 1 + \mathcal{O}(\tau_x^{8\alpha}),$$

as soon as  $\tau_x < (C' \mathcal{E}_{H, \min})^{-1/2\alpha}$ .

The function  $u_1 = \|\tilde{\chi}_1 u_0\|_{L^2}^{-1} \tilde{\chi}_1 u_0$  is normalized with

$$\mathcal{E}_{H, \min} \leq \mathcal{E}_H(u_1) \leq \mathcal{E}_{H, \min} + \mathcal{O}(\tau_x^{6\alpha}),$$

and  $\chi_1(\tau_x^\alpha)u_1 = u_1$ ,  $\chi_2(\tau_x^\alpha)u_1 = 0$ . Applying the second formula of Lemma 4.5 with, now, the pair  $\chi$ , leads to

$$\begin{aligned} \mathcal{E}_\tau(u_1) &= \mathcal{E}_H(u_1) + R(u_1) = \mathcal{E}_{H,min} + \mathcal{O}(\tau_x^{6\alpha}) + R(u_1) \\ \text{with } R(u_1) &\leq \frac{1}{4}(\mathcal{E}_\tau(u_1))^{1/2} + (\mathcal{E}_{H,min} + \mathcal{O}(\tau_x^{6\alpha}))^{1/2}\tau_x^{1-3\alpha}. \end{aligned}$$

With the estimate  $\frac{\sqrt{2}}{2} \leq \mathcal{E}_{H,min} \leq C$ , we deduce

$$\mathcal{E}_\tau(u_1) = \mathcal{E}_{H,min} + \mathcal{O}(\tau_x^{6\alpha} + \tau_x^{1-3\alpha}).$$

It's time to fix  $\alpha$  to the value  $\frac{1}{9}$  so that  $\tau_x^{6\alpha} = \tau_x^{1-3\alpha} = \tau_x^{2/3}$  and

$$\inf_{u \in H^1(\mathbb{R}^2)} \mathcal{E}_\tau(u) \leq \mathcal{E}_\tau(u_1) \leq \mathcal{E}_{H,min} + \kappa\tau_x^{2/3}.$$

Second step - Existence of a minimizer: Once the function  $u_1 \in H^1(\mathbb{R}^2)$  has been constructed as above, consider  $\tau_x < \tau_0$  with  $\mathcal{E}_{H,min} + \kappa\tau_0^{2/3} \leq \frac{1}{\ell_V^2\tau_0}$ . The functional

$$\mathcal{E}_\tau(u) - \frac{1}{\ell_V^2\tau_x}\|u\|_{L^2}^2,$$

is the sum of a convex strongly continuous functional (and therefore weakly continuous) on  $H^1(\mathbb{R}^2)$  and a negative functional

$$\langle u, \frac{1}{\ell_V^2\tau_x} [v(\tau_x^{1/2}.) - 1]_- u \rangle.$$

Due to the compact support of  $v-1$ , it is also continuous w.r.t the weak topology on  $H^1(\mathbb{R}^2)$ . Out a minimizing sequence  $(u_n)_{n \in \mathbb{N}^*}$ , extract a weakly converging subsequence in  $H^1(\mathbb{R}^2)$ . The weak limit,  $u_\infty$ , satisfies

$$\mathcal{E}_\tau(u_\infty) - \frac{1}{\ell_V^2\tau_x}\|u_\infty\|_{L^2}^2 = \lim_{k \rightarrow \infty} \mathcal{E}_\tau(u_{n_k}) - \frac{1}{\ell_V^2\tau_x}\|u_{n_k}\|_{L^2}^2.$$

with  $\|u_\infty\|_{L^2} \leq 1$ . The same convergence holds also for the energy  $\mathcal{E}_\tau(u) - \frac{1}{2\ell_V^2\tau_x}\|u\|_{L^2}^2$ , so that actually  $\|u_\infty\|_{L^2} = \lim_{k \rightarrow \infty} \|u_{n_k}\|_{L^2} = 1$  and  $u_\infty$  realizes the minimum of  $\mathcal{E}_\tau(u)$  under the constraint  $\|u\|_{L^2} = 1$ .

The Euler-Lagrange equation can thus be written, with the stated straightforward consequences.

Third step - a priori estimate for minimizers of  $\mathcal{E}_\tau$ :

Let  $u \in H^1(\mathbb{R}^2)$  satisfy  $\|u\|_{L^2} = 1$  and  $\mathcal{E}_\tau(u) = \mathcal{E}_{\tau,min} \leq \mathcal{E}_H + \kappa\tau_x^{2/3}$ . Take two pairs  $\tilde{\chi} = (\tilde{\chi}_1, \tilde{\chi}_2)$  and  $\chi' = (\chi'_1, \chi'_2)$ , like in our statement, and such that  $\chi'_1 \prec \tilde{\chi}_1$ . The identities (4.9) for  $\mathcal{E}_\tau$  and (4.9) in Lemma 4.5 provide

$$\begin{aligned} \mathcal{E}_{\tau,min} &\geq \mathcal{E}_\tau(\tilde{\chi}_1(\tau_x^{1/9}.)u) - C_{\tilde{\chi}}\tau_x^{2/9} \\ \mathcal{E}_{\tau,min} &\geq \mathcal{E}_H(\tilde{\chi}_1(\tau_x^{1/9}.)u) - C_{\tilde{\chi}}\tau_x^{2/9} \\ &\quad - \frac{1}{4} \left[ \mathcal{E}_\tau(\tilde{\chi}_1(\tau_x^{1/9}.)u)^{1/2} + \mathcal{E}_H(\tilde{\chi}_1(\tau_x^{1/9}.)u)^{1/2} \right] \tau_x^{2/3}. \end{aligned}$$

The first line says

$$\mathcal{E}_\tau(\tilde{\chi}_1(\tau_x^{1/9}.)u) \leq \mathcal{E}_{\tau,min} + C_{\tilde{\chi}}\tau_x^{2/9} \leq \mathcal{E}_{H,min} + \kappa\tau_x^{2/3} + C_{\tilde{\chi}}\tau_x^{2/9} \leq C'_{\tilde{\chi}},$$

which combined with the second line provides the uniform estimate

$$\mathcal{E}_\tau(\tilde{\chi}_1(\tau_x^{1/9}.)u) \leq C''_{\tilde{\chi}}.$$

Therefore  $\tilde{\chi}_1(\tau_x^{1/9}.)u$  is uniformly bounded in  $\mathcal{H}_1$  with respect to  $\tau_x$ . Consider now the Euler-Lagrange equation

$$\left[ -\partial_x^2 - \left( \partial_y - \frac{i}{2} \frac{x}{\sqrt{1+\tau_x x^2}} \right)^2 + \frac{v(\tau_x^{1/2}.)}{\ell_V^2 \tau_x} + G|u|^2 \right] u = \lambda_u u$$

and write its local version for  $u'_1 = \chi'_1(\tau_x^{2/9}.)u$  in the form

$$\begin{aligned} \left[ -\partial_x^2 - \left( \partial_y - \frac{ix}{2} \right)^2 + \frac{x^2 + y^2}{\ell_V^2} \right] u'_1 &= \lambda_u u'_1 - G|\tilde{u}_1|^2 u'_1 \\ &\quad + f_u^1 + f_u^2, \end{aligned} \quad (4.14)$$

with  $f_u^1 = -ix \left( \frac{1}{\sqrt{1+\tau_x x^2}} - 1 \right) \chi'_1(\tau_x^{1/9}.) \partial_y \tilde{u}_1 - \frac{x^2}{4} \frac{\tau_x x^2}{1+\tau_x x^2} u'_1,$

and  $f_u^2 = -2\tau_x^{1/9} (\nabla \chi'_1)(\tau_x^{1/9}.) \cdot \nabla \tilde{u}_1 - \tau_x^{2/9} (\Delta \chi'_1)(\tau_x^{1/9}.) \tilde{u}_1,$

after setting  $\tilde{u}_1 = \tilde{\chi}_1(\tau_x^{2/9}.)u$ . Both functions,  $\tilde{u}_1$  and therefore  $u'_1 = \chi'_1(\tau_x^{2/9}.)\tilde{u}_1$  are uniformly estimated in  $\mathcal{H}_1$  and therefore in  $H^1(\mathbb{R}^2)$ . From the embedding  $H^1(\mathbb{R}^2) \subset L^6(\mathbb{R}^2)$ , the term  $G|\tilde{u}_1|^2 u'_1$  is uniformly bounded in  $L^2(\mathbb{R}^2)$ . For the term  $f_u^1$ , the support condition  $\text{supp } \chi'_1(\tau_x^{1/9}.) \subset \{|x| \leq \tau_x^{-1/9}\}$  imply

$$\|f_u^1\|_{L^2} \leq C_{\chi'}(\tau_x^{1-1/3} + \tau_x^{1-4/9}) \leq C''_{\chi'},$$

while the estimate

$$\|f_u^2\| \leq C_{\chi'} \tau_x^{1/9} \leq C''_{\chi'}$$

is straightforward. Hence the right-hand side of (4.14) is uniformly bounded in  $L^2(\mathbb{R}^2)$  and we have proved

$$\|\chi'_1(\tau_x^{1/9}.)u\|_{\mathcal{H}_2} \leq C_{\chi'}^3 \quad (4.15)$$

for any good pair of cut-offs  $\chi' = (\chi'_1, \chi'_2)$ .

Fourth step- accurate comparison of minimal energies:

We already know  $\mathcal{E}_{\tau,min} \leq \mathcal{E}_{H,min} + \kappa\tau_x^{2/3}$  and we want to check the reverse inequality. Consider a minimizer  $u$  of  $\mathcal{E}_\tau$  and take two pairs of cut-off  $\chi = (\chi_1, \chi_2)$  and  $\chi' = (\chi'_1, \chi'_2)$ , such that  $\chi_1 \prec \chi'_1$ . The identity (4.8) for  $\mathcal{E}_\tau$  and

(4.9) of Lemma 4.5 used with  $\chi$  imply

$$\begin{aligned} \mathcal{E}_{\tau, \min} &\geq \mathcal{E}_{\tau}(\chi_1(\tau_x^{1/9} \cdot)u) + \mathcal{E}_{\tau}(\chi_2(\tau_x^{1/9} \cdot)u) \\ &\quad - \tau_x^{2/9} \sum_{j=1}^2 \int_{\mathbb{R}^2} |(\nabla \chi_j)(\tau_x^{1/9} \cdot)|^2 |u|^2, \end{aligned} \quad (4.16)$$

$$\begin{aligned} \mathcal{E}_{\tau, \min} &\geq \mathcal{E}_H(\chi_1(\tau_x^{1/9} \cdot)u) \\ &\quad - \tau_x^{2/9} \sum_{j=1}^2 \int_{\mathbb{R}^2} |(\nabla \chi_j)(\tau_x^{1/9} \cdot)|^2 |u|^2 + R(u). \end{aligned} \quad (4.17)$$

After setting  $u'_1 = \chi'_1(\tau_x^{1/9} \cdot)u$ , we get the bound

$$\int_{\mathbb{R}^2} |(\nabla \chi_j)(\tau_x^{1/9} \cdot)|^2 |u|^2 = \int_{\mathbb{R}^2} \frac{|(\nabla \chi_j)(\tau_x^{1/9} \cdot)|^2}{|q|^4} \|q\|^2 u'_1|^2 \leq C_{\chi} \tau_x^{4/9},$$

while we already know from the third step the bounds  $\mathcal{E}_{\bullet}(\chi_1(\tau_x^{1/9} \cdot)u) \leq C_{\chi}$  when  $\bullet$  stands for  $\tau$  or  $H$ , which implies  $|R(u)| \leq C_{\chi} \tau_x^{2/3}$ . From (4.16), we deduce, as we did in the first step with the energy  $\mathcal{E}_H$ ,

$$\|\chi_2(\tau_x^{1/9} \cdot)u\|_{L^2}^2 \leq C_{\chi} \tau_x^{2/3} \quad , \quad \|\chi_1(\tau_x^{1/9} \cdot)u\|_{L^2} = 1 + \mathcal{O}(\tau_x^{2/3}),$$

while the second line implies

$$\mathcal{E}_{\tau, \min} \geq \left(1 - C_{\chi} \tau_x^{2/3}\right) \mathcal{E}_{H, \min} - C'_{\chi} \tau_x^{2/3} \geq \mathcal{E}_{H, \min} - C''_{\chi} \tau_x^{2/3}.$$

Fifth step- accurate comparison of minimizers:

The function  $u_1 = \|\chi_1(\tau_x^{1/9} \cdot)u\|_{L^2}^{-1} \chi_1(\tau_x^{1/9} \cdot)u$ , satisfies

$$\mathcal{E}_H(u_1) \leq \mathcal{E}_{H, \min} + C_{\chi} \tau_x^{2/3}$$

while  $\chi_1(\tau_x^{1/9} \cdot)u$  solves the equation (4.14) for some pair  $\tilde{\chi} = (\tilde{\chi}_1, \tilde{\chi}_2)$  such that  $\chi_1 \prec \tilde{\chi}_1$  after replacing  $(\chi', u'_1)$  with  $(\chi, \chi_1(\tau_x^{1/9} \cdot)u)$ . After normalization by setting  $\tilde{u}_1 = \|\chi(\tau_x^{1/9} \cdot)u\|_{L^2}^{-1} \chi_1(\tau_x^{1/9} \cdot)u$  it becomes

$$\begin{aligned} H_{\ell_V, G} u_1 + G|u_1|^2 u_1 &= \lambda_u u_1 + f_u^1 + f_u^2 + f_u^3, \\ u_1 &= \|\chi(\tau_x^{1/9} \cdot)u\|_{L^2}^{-1} \chi_1(\tau_x^{1/9} \cdot)u \quad , \quad \tilde{u}_1 = \|\chi(\tau_x^{1/9} \cdot)u\|_{L^2}^{-1} \tilde{\chi}_1(\tau_x^{1/9} \cdot)u, \\ \text{with} \quad f_u^1 &= -ix \left( \frac{1}{\sqrt{1 + \tau_x x^2}} - 1 \right) \chi(\tau_x^{1/9} \cdot) \partial_y \tilde{u}_1 - \frac{x^2}{4} \frac{\tau_x x^2}{1 + \tau_x x^2} u_1, \\ f_u^2 &= -2\tau_x^{1/9} (\nabla \chi_1)(\tau_x^{1/9} \cdot) \cdot \nabla \tilde{u}_1 - \tau_x^{2/9} (\Delta \chi_1)(\tau_x^{1/9} \cdot) \tilde{u}_1, \\ \text{and} \quad f_u^3 &= G \|\chi_1(\tau_x^{1/9} \cdot)u\|_{L^2}^2 (|\tilde{u}_1|^2 - |u_1|^2) u_1 + G(1 - \|\chi_1(\tau_x^{1/9} \cdot)u\|_{L^2}^2) |u_1|^2 u_1. \end{aligned} \quad (4.18)$$

The estimate (4.15), for any new good pair  $\chi' = (\chi'_1, \chi'_2)$  such that  $\chi_1 \prec \tilde{\chi}_1 \prec \chi'_1$ , implies that the terms  $f_u^1$  and  $f_u^2$  of the right-hand side of (4.18) have



an  $L^2$ -norm of order  $\tau_x^{2/3}$ . For the third term the estimate (4.15) also implies that

$$(|\tilde{u}_1|^2 - |u_1|^2)u_1 = \left(1 - \chi_1^2(\tau_x^{1/9}.)\right) |\tilde{u}_1|^2 u_1,$$

has an  $L^2$ -norm of order  $\mathcal{O}(\tau_x^{2/3})$  (use the  $L^\infty$  bound for  $|\tilde{u}_1|^2$  with  $\| |q|^2 u_1 \|_{L^2} \leq C_\chi$ ). We conclude by applying Proposition 4.4.  $\square$

We end this section with a comparison property similar to Proposition 4.4.

**Proposition 4.7.** *Let  $\ell_V, G$  be fixed positive numbers and take  $u \in H^1(\mathbb{R}^2)$  such that*

$$\mathcal{E}_\tau(u) \leq \mathcal{E}_{\tau, \min} + C_{\ell_V, G} \tau_x^{2/3}$$

*and which solves*

$$-\partial_x^2 u - \left(\partial_y - i \frac{x}{\sqrt{1 + \tau_x x^2}}\right)^2 u + \frac{v(\tau_x^{1/2}.)}{\ell_V^2 \tau_x} u + G|u|^2 u = \lambda_u u + r_u$$

*with  $\lambda_u \in \mathbb{R}$  and  $\|r_u\|_{L^2} \leq 1$ . Then for any pair  $\chi = (\chi_1, \chi_2) \in \mathcal{C}_b^\infty(\mathbb{R}^2)$  so that  $\chi_1^2 + \chi_2^2 = 1$  with  $\text{supp } \chi_1 \subset \{x^2 + y^2 < 1\}$  and  $\chi_1 \equiv 1$  in  $\{x^2 + y^2 \leq 1/2\}$ , there exists  $\tau_{\chi, \ell_V, G}$  and  $C_{\chi, \ell_V}$  such that*

$$\|\chi_2(\tau_x^{1/9}.)u\|_{L^2}^2 \leq C_{\chi, \ell_V, G} \tau_x^{2/3} \quad (4.19)$$

$$|\mathcal{E}_\tau(\chi_1(\tau_x^{1/9}.)u) - \mathcal{E}_{H, \min}| \leq C_{\chi, \ell_V, G} \tau_x^{2/3} \quad (4.20)$$

$$d_{\mathcal{H}_2}(\chi_1(\tau_x^{1/9}.)u, \text{Argmin } \mathcal{E}_H) \leq C_{\chi, \ell_V, G} (\tau_x^{2\nu_{\ell_V, G}/3} + \|r_u\|_{L^2}), \quad (4.21)$$

*when  $\tau_x < \tau_{\chi, \ell_V, G}$  and where  $\nu_{\ell_V, G} \in (0, \frac{1}{2}]$  is the exponent given in Proposition 4.2.*

**Proof:** The analysis follows essentially the same line as the study of the minimizers of  $\mathcal{E}_\tau$  in the proof of Proposition 4.6. By taking two pairs  $\chi' = (\chi'_1, \chi'_2)$  and  $\tilde{\chi} = (\tilde{\chi}_1, \tilde{\chi}_2)$  such that  $\chi'_1 \prec \tilde{\chi}_1$ , we obtain successively like in the Third Step in the proof of Proposition 4.6 :

- $\mathcal{E}_\tau(\tilde{\chi}_1(\tau_x^{1/9}.)u) + \mathcal{E}_\tau(\tilde{\chi}_2(\tau_x^{1/9}.)u) \leq C_{\tilde{\chi}}$ ;
- $\left[-\partial_x^2 - \left(\partial_y - \frac{ix}{2}\right)^2 + \frac{x^2 + y^2}{\ell_V^2}\right] u'_1 = \lambda_u u'_1 - G|\tilde{u}_1|^2 u'_1 + f_u^1 + f_u^2 + r_u$  where  $u'_1, \tilde{u}_1, f_u^{1,2}$  have the same expressions as in (4.14);
- $\|\chi'_1(\tau_x^{1/9}.)u\|_{\mathcal{H}_2} \leq C_{\chi'}$  owing to  $\|r_u\|_{L^2} \leq 1$ .

From the last estimate, the refined comparison of energies like in the Fourth Step gives for a pair  $\chi = (\chi_1, \chi_2)$  such that  $\chi_1 \prec \chi'_1$ :

$$\|\chi_2(\tau_x^{1/9}.)u\|_{L^2}^2 \leq C_\chi \tau_x^{2/3} \quad \mathcal{E}_H(u_1) \leq \mathcal{E}_{H, \min} + C_\chi \tau_x^{2/3},$$

with  $u_1 = \|\chi_1(\tau_x^{1/9}.)u\|^{-1} \chi_1(\tau_x^{1/9}.)u$  and  $C_\chi \tau_x^{2/3} \leq 1$  for  $\tau_x \leq \tau_\chi$ . The equation (4.18) is replaced by

$$H_{\ell_V, G} u_1 + G|u_1|^2 u_1 = \lambda_u u_1 + f_u^1 + f_u^2 + f_u^3 + \|\chi_1(\tau_x^{1/9}.)u\|^{-1} r_u$$

without changing the expressions of  $f_u^{1,2,3}$ . Again the estimate  $\|\chi'_1(\tau_x^{1/9}.)u\|_{\mathcal{H}_2} \leq C_{\chi'}$  is used with various cut-offs  $\chi'_1$ , in order to get  $\|f_u^1 + f_u^2 + f_u^3\|_{L^2} = \mathcal{O}(\tau_x^{2/3})$ . We conclude with the help of Proposition 4.4 applied to  $u_1$ .  $\square$

## 5 Analysis of the complete minimization problem

We consider the complete minimization problem for the energy

$$\mathcal{E}_\varepsilon(\psi) = \langle \psi, H_{Lin} \psi \rangle + \frac{G_{\varepsilon,\tau}}{2} \int |\psi|^4 = \varepsilon^{2+2\delta} \tau_x \left[ \langle \psi, \varepsilon^{-2-2\delta} \tau_x^{-1} H_{Lin} \psi \rangle + \frac{G}{2} \int |\psi|^4 \right]$$

and compare its solutions to the minimization of the reduced energies  $\mathcal{E}_\tau$  and  $\mathcal{E}_H$ , introduced in the previous sections. We work with  $\tau_y = 1$ ,  $\tau_x \rightarrow 0$ ,  $\varepsilon \rightarrow 0$ , while  $\ell_V, G$  and  $\delta \in (0, \delta_0]$  are fixed. The analysis follows the same lines as the proof of Proposition 4.6.

### 5.1 Upper bound for $\inf \{\mathcal{E}_\varepsilon(\psi), \|\psi\|_{L^2} = 1\}$

The potential  $V_\varepsilon$  is chosen according to (1.13)-(1.14) while  $\ell_V$  and  $G$  are fixed. The parameter  $\tau_x$  is assumed to be smaller than  $\tau_{\ell_V, G}$  so that the minimal energy  $\mathcal{E}_{\tau, \min}(\tau_x)$  of  $\mathcal{E}_\tau$  is achieved (see Proposition 4.6) and  $|\mathcal{E}_{\tau, \min}(\tau_x) - \mathcal{E}_{H, \min}| \leq C_{\ell_V, G} \tau_x^{2/3}$ . Moreover Proposition 4.6 also says that by truncating an element of Argmin  $\mathcal{E}_\tau$ , one can find  $a_- \in \mathcal{H}_2$  such that

$$\|a_-\|_{L^2} = 1, \quad |\mathcal{E}_\tau(a_-) - \mathcal{E}_{H, \min}| \leq C_{\ell_V, G} \tau_x^{2/3} \quad \text{and} \quad \|a_-\|_{\mathcal{H}_2} \leq C_{\ell_V, G}. \quad (5.1)$$

**Proposition 5.1.** *Under the above assumptions, take  $\psi = \hat{U} \begin{pmatrix} 0 \\ e^{-i \frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$*

*where  $a_-$  satisfies (5.1) and  $\hat{U} = U(q, \varepsilon D_q, \tau, \varepsilon)$  is the unitary operator introduced in Theorem 2.1. The estimate*

$$|\mathcal{E}_\varepsilon(\psi) - \varepsilon^{2+2\delta} \tau_x \mathcal{E}_\tau(a_-)| \leq C_{\ell_V, G} \varepsilon^{2+4\delta}. \quad (5.2)$$

*hold uniformly w.r.t  $\tau_x \in (0, \tau_{\ell_V, G}]$  and  $\delta \in (0, \delta_0]$ .*

**Proof:** Let us compare first the linear part by estimating

$$\begin{aligned} \left| \langle \psi, H_{Lin} \psi \rangle - \varepsilon^{2+2\delta} \tau_x \langle a_-, \left[ -\partial_x^2 - (\partial_y - i \frac{x}{2\sqrt{1+\tau_x x^2}})^2 + \frac{v(\sqrt{\tau_x}.)}{\ell_V^2 \tau_x} \right] a_- \rangle \right| \\ = |\langle \psi, (H_{Lin} - \varepsilon^{2+2\delta} \tau_x U^* H_{BO} U) \psi \rangle| \end{aligned}$$

By Proposition 3.2, it suffices to estimate

$$\|(1 - \hat{\chi})\psi\|_{L^2} \quad \text{and} \quad \|\sqrt{\tau_x} |\varepsilon D_q| (1 - \hat{\chi})\psi\|_{L^2}$$

for some given cut-off function  $\chi \in C_0^\infty(\mathbb{R})$  with  $\hat{\chi} = \chi(\tau_x \varepsilon^2 D_q^2)$ . Notice

$$e^{i\frac{y}{2\sqrt{\tau_x}}}(\sqrt{\tau_x}\varepsilon D_q)e^{-i\frac{y}{2\sqrt{\tau_x}}} = \begin{pmatrix} \sqrt{\tau_x}\varepsilon D_x \\ \sqrt{\tau_x}\varepsilon D_y - \frac{\varepsilon}{2} \end{pmatrix}$$

Hence by using the functional calculus of  $\sqrt{\varepsilon}D_q$ , we can say that there exists a cut-off  $\chi' \in C_0^\infty(-r_\gamma^2, r_\gamma^2)$ , with  $\chi' \equiv 1$  around 0 and  $\chi' \prec \chi$  such that

$$e^{i\frac{y}{2\sqrt{\tau_x}}}(1 - \hat{\chi})^2 e^{-i\frac{y}{2\sqrt{\tau_x}}} \leq (1 - \hat{\chi}')^2,$$

$$\text{and } e^{i\frac{y}{2\sqrt{\tau_x}}}(\tau_x \varepsilon^2 |D_q|^2)(1 - \hat{\chi})^2 e^{-i\frac{y}{2\sqrt{\tau_x}}} \leq 2(\tau_x \varepsilon^2 |D_q|^2)(1 - \hat{\chi}')^2 + 2(1 - \hat{\chi}')^2$$

as soon as  $\varepsilon \leq \varepsilon_0 \leq 1$ , for a convenient choice of  $\varepsilon_0$  and  $r_\gamma$ . By using  $\|a\|_{H^2(\mathbb{R}^2)} \leq C_{\ell_V, G}$ , we deduce

$$\|(1 - \hat{\chi})\psi\|_{L^2}^2 \leq \|(1 - \hat{\chi}')a_-\|_{L^2}^2 \leq C_{\ell_V, G} \tau_x^2 \varepsilon^4,$$

and

$$\begin{aligned} \|(\sqrt{\tau_x}\varepsilon |D_q|)(1 - \hat{\chi})\psi\|_{L^2}^2 &\leq 2\|(\sqrt{\tau_x}\varepsilon |D_q|)(1 - \hat{\chi}')a_-\|_{L^2}^2 + 2\|(1 - \hat{\chi}')a_-\|_{L^2}^2 \\ &\leq C_{\ell_V, G} \tau_x \varepsilon^2. \end{aligned}$$

By Proposition 3.2, we obtain

$$\begin{aligned} &|\langle \psi, (H_{Lin} - \varepsilon^{2+2\delta} \tau_x U^* H_{BO} U) \psi \rangle| \\ &\leq C_{\ell_V, G} \left[ \varepsilon^{2+4\delta} + \varepsilon^{5+2\delta} \tau_x^2 + \varepsilon^{4+2\delta} \tau_x^{3/2} \right] \leq C'_{\ell_V, G} \varepsilon^{2+4\delta}. \end{aligned} \quad (5.3)$$

For the nonlinear part of the energy, Proposition 3.3 gives

$$(1 - C\varepsilon^{1+2\delta}) \int_{\mathbb{R}^2} |a_-|^4 \leq \int_{\mathbb{R}^2} |\psi|^4 \leq (1 + C\varepsilon^{1+2\delta}) \int_{\mathbb{R}^2} |a_-|^4$$

and the bound,  $\int_{\mathbb{R}^2} |e^{-i\frac{y}{2\sqrt{\tau_x}}} a_-|^4 = \int_{\mathbb{R}^2} |a_-|^4 \leq C_{\ell_V, G}$ , leads to

$$\left| \frac{G\tau_x \varepsilon^{2+2\delta}}{2} \int_{\mathbb{R}^2} |\psi|^4 - \varepsilon^{2+2\delta} \frac{G\tau_x}{2} \int_{\mathbb{R}^2} |a_-|^4 \right| \leq C_{\ell_V, G} \varepsilon^{2+2\delta} \tau_x \times \varepsilon^{1+2\delta},$$

which is smaller than the error term for the linear part. This ends the proof of (5.2).  $\square$

**Remark 5.2.** • The energy  $\mathcal{E}_\tau(a_-) = \mathcal{E}_{H, \min} + \mathcal{O}(\tau_x^{2/3})$ . Therefore the error given by (5.2) is relevant, as compared with the energy scale of  $\varepsilon^{2+2\delta} \tau_x \mathcal{E}_{\tau, \min}$ , when

$$\varepsilon^{2\delta} \leq c_{\ell_V, G} \tau_x, \quad (5.4)$$

with  $c_{\ell_V, G}$  small enough, and accurate when

$$\varepsilon^{2\delta} \leq C_{\ell_V, G} \tau_x^{5/3}. \quad (5.5)$$

Remember that the constants  $c_{\ell_V, G}$  and  $C_{\ell_V, G}$  depend also on  $\delta_0$ , when  $\delta \in (0, \delta_0]$ .

- It is interesting to notice that the worst term in the right-hand side of (5.3) comes from the error of order  $\mathcal{O}(\varepsilon^{2+2\delta})$  in the Born-Oppenheimer approximation. There seems to be no way to get an additional factor  $\tau_x^\alpha$  with  $\alpha > 0$  because the initial problem is rapidly oscillatory in the  $y$ -variable in a  $\tau_x$ -dependent scale. This can be seen on the gain associated with the metric  $g_\tau$ , for  $\tau_y = 1$  and  $\tau_x > 0$ , which is simply  $\langle \sqrt{\tau_x} p \rangle$  or essentially 1 when  $p$  is small.

## 5.2 Existence of a minimizer for $\mathcal{E}_\varepsilon$

With the choice (1.13)-(1.14) of the potential  $V_{\varepsilon,\tau}$ , the linear Hamiltonian  $H_{Lin}$  can be written

$$H_{Lin} = -\varepsilon^{2+2\delta}\tau_x\Delta + u_0(q, \tau) \begin{pmatrix} 2\sqrt{1+\tau_x x^2} & 0 \\ 0 & 0 \end{pmatrix} u_0(q, \tau)^* \\ + \varepsilon^{2+2\delta} \frac{v(\tau_x^{1/2} \cdot)}{\ell_V^2} - \varepsilon^{2+2\delta} W_\tau(x, y),$$

$$\text{with } W_\tau(x, y) = \frac{\tau_x^2}{(1+\tau_x x^2)^2} + \frac{1}{1+\tau_x x^2}.$$

For  $t \leq \frac{\varepsilon^{2+2\delta}}{2\ell_V^2}$ , the negative part  $\left( \varepsilon^{2+2\delta} \frac{v(\sqrt{\tau_x} \cdot)}{\ell_V^2} - t \right)_-$  is compactly supported. Set

$$H_{Lin,t,+} = -\varepsilon^{2+2\delta}\tau_x\Delta + u_0(q, \tau) \begin{pmatrix} 2\sqrt{1+\tau_x x^2} & 0 \\ 0 & 0 \end{pmatrix} u_0(q, \tau)^* \\ + \left( \varepsilon^{2+2\delta} \frac{v(\sqrt{\tau_x} \cdot)}{\ell_V^2} - t \right)_+,$$

so that

$$\mathcal{E}_\varepsilon(\psi) - t\|\psi\|^2 = \langle \psi, H_{Lin,t,+} \psi \rangle + \frac{G_{\varepsilon,\tau}}{2} \int |\psi|^4 \\ + \langle \psi, \varepsilon^{2+2\delta} \left[ \left( \frac{v(\sqrt{\tau_x} \cdot)}{\ell_V^2} - \frac{t}{\varepsilon^{2+2\delta}} \right)_- - W_\tau \right] \psi \rangle. \quad (5.6)$$

**Proposition 5.3.** Assume  $\varepsilon \leq \varepsilon_{\ell_V,G}$  and  $\tau_x \leq \tau_{\ell_V,G}$  with  $\tau_{\ell_V,G}$  small enough. Then the infimum

$$\inf \{ \mathcal{E}_\varepsilon(u), \quad u \in H^1(\mathbb{R}^2), \|u\|_{L^2} = 1 \}$$

is achieved. Any element  $\psi$  of Argmin  $\mathcal{E}_\varepsilon$  solves an Euler-Lagrange equation

$$H_{Lin}\psi + G_{\varepsilon,\tau}|\psi|^2\psi = \lambda_\psi\psi$$

with the estimates

$$|\mathcal{E}_\varepsilon(\psi)| + |\lambda_\psi| \leq C_{\ell_V,G} \varepsilon^{2+2\delta}, \quad \|(1+\tau_x|D_q|^2)^{1/2}\psi\|_{L^2} \leq C_{\ell_V,G}, \\ \mathcal{E}_\varepsilon(\psi) = \mathcal{E}_{\varepsilon,min} \leq \varepsilon^{2+2\delta} \left[ \mathcal{E}_{\tau,min} + C_{\ell_V,G} \varepsilon^{2\delta} \right] \\ \leq \varepsilon^{2+2\delta} \left[ \tau_x \mathcal{E}_{H,min} + C'_{\ell_V,G} (\tau_x^{5/3} + \varepsilon^{2\delta}) \right].$$

**Proof:** From Proposition 5.1, we know that

$$\inf_{\|u\|_{L^2}=1} \mathcal{E}_\varepsilon(u) \leq \varepsilon^{2+2\delta} \tau_x \mathcal{E}_{\tau,min} + C_{\ell_V,G} \varepsilon^{2+4\delta} =: \frac{t}{2}.$$

For  $\varepsilon \leq \varepsilon_{\ell_V,G}$  and  $\tau_x \leq \tau_{\ell_V,G}$ ,  $t$  smaller than  $\frac{\varepsilon^{2+2\delta}}{2\ell_V^2}$ . Consider the decomposition (5.6) for the energy  $\mathcal{E}_\varepsilon(u) - t\|u\|_{L^2}^2$ . By the same argument (convexity of the positive part and compactness of the negative part) as we used for  $\mathcal{E}_\tau$  in the proof of Proposition 4.6 (second step), a weak limit of an extracted sequence of minimizers in  $H^1(\mathbb{R}^2)$  is a minimum for  $\mathcal{E}_\varepsilon$  on  $\{\|u\|_{L^2} = 1\}$ .

A element  $\psi$  of Argmin  $\mathcal{E}_\varepsilon$  satisfies

$$\begin{aligned} \varepsilon^{2+2\delta} \tau_x \left[ \langle \psi, -\Delta \psi \rangle + \frac{G}{2} \int |\psi|^4 \right] &\leq \langle \psi, H_{Lin,t,+} \psi \rangle + \frac{G_{\varepsilon,\tau}}{2} \int |\psi|^4 \\ &\leq \mathcal{E}_{\varepsilon,min} - \langle \psi, \varepsilon^{2+2\delta} \left[ \left( \frac{v(\sqrt{\tau_x \cdot})}{\ell_V^2} - \frac{t}{\varepsilon^{2+2\delta}} \right)_- - W_\tau \right] \psi \rangle \\ &\leq \frac{t}{2} + t + (1 + \tau_x^2) \varepsilon^{2+2\delta} \leq C'_{\ell_V,G} \varepsilon^{2+2\delta}, \end{aligned}$$

by recalling  $v \geq 0$  for the last line. This implies

$$\|\psi\|_{H^1}^2 \leq C'_{\ell_V,G} \tau_x^{-1}, \quad \|\psi\|_{L^4}^4 \leq \frac{2C'_{\ell_V,G}}{G} \tau_x^{-1},$$

and by interpolation with  $\|u\|_{L^6} \leq C \|\nabla u\|_{L^2}^{2/3} \|u\|_{L^2}^{1/3}$ ,  $\|\psi\|_{L^6} = \mathcal{O}(\tau_x^{-1/3})$ . The first inequality with  $\|\psi\|_{L^2} = 1$ , gives  $\|(1 + \tau_x |D_q|^2)^{1/2} \psi\|_{L^2} = \mathcal{O}(1)$ . The Euler-Lagrange equation

$$H_{Lin} \psi + G_{\varepsilon,\tau} |\psi|^2 \psi = \lambda \psi$$

implies

$$\begin{aligned} |\lambda| &\leq 2 \left[ \langle \psi, H_{Lin,t,+} \psi \rangle + \frac{G_{\varepsilon,\tau}}{2} \int |\psi|^4 \right] \\ &\quad - \langle \psi, \varepsilon^{2+2\delta} \left[ \left( \frac{v(\sqrt{\tau_x \cdot})}{\ell_V^2} - \frac{t}{\varepsilon^{2+2\delta}} \right)_- - W_\tau \right] \psi \rangle \leq C''_{\ell_V,G} \varepsilon^{2+2\delta}. \end{aligned}$$

Similarly, the lower bound  $\mathcal{E}_\varepsilon(\psi) \geq -2\varepsilon^{2+2\delta}$  is due to  $W_\tau \geq -2$ . The upper bound of  $\mathcal{E}_\varepsilon(\psi) = \mathcal{E}_{\varepsilon,min}$  comes from Proposition 5.1 and (5.1).  $\square$

### 5.3 Comparison of minimal energies between $\mathcal{E}_\varepsilon$ and $\mathcal{E}_\tau$

In this subsection, we specify a priori estimates for the minimizers of  $\mathcal{E}_\varepsilon$  and compare the energies  $\mathcal{E}_{\varepsilon,min}$  and  $\mathcal{E}_{\tau,min}$  without imposing relations between  $\varepsilon^{2\delta}$  and  $\tau_x$ . This is not necessary at this level, if one uses carefully bootstrap arguments.

**Proposition 5.4.** *Let  $V_{\varepsilon,\tau}$  be given by (1.13)-(1.14) and assume  $\tau_x \leq \tau_{\ell_V,G}$  and  $\varepsilon \leq \varepsilon_{\ell_V,G}$  so that  $\mathcal{E}_\varepsilon$  admits a ground state according to Proposition 5.3. The operator  $\hat{U}$  is the unitary transform provided by Theorem 2.1 and an element  $\psi \in \text{Argmin } \mathcal{E}_\varepsilon$  is written  $\hat{U} \begin{pmatrix} e^{+i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$ , with  $a = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}$ . Then, the estimates*

$$\|(1 + \tau_x |D_q|^2)^{1/2} a\|_{L^2} \leq C_{\ell_V,G}, \quad (5.7)$$

$$\|a_+\|_{L^2}^2 + G_{\varepsilon,\tau} \int |a|^4 \leq C_{\ell_V,G} \varepsilon^{2+4\delta} + \mathcal{E}_{\varepsilon,min}, \quad (5.8)$$

$$|\mathcal{E}_\varepsilon(\psi) - \varepsilon^{2+2\delta} \tau_x \mathcal{E}_\tau(a_-)| \leq C_{\ell_V,G} \varepsilon^{2+4\delta}, \quad (5.9)$$

$$|\mathcal{E}_{\varepsilon,min} - \varepsilon^{2+2\delta} \tau_x \mathcal{E}_{\tau,min}| \leq C_{\ell_V,G} \varepsilon^{2+4\delta}, \quad (5.10)$$

hold with right-hand sides which can be replaced by  $C_{\ell_V,G} \varepsilon^{2+2\delta} \tau_x$  when  $\varepsilon^{2\delta} \leq C_{\ell_V,G} \tau_x$ .

**Proof:** For  $\tilde{a} = \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$  and  $a = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}$ , the norms  $\|(1 + \tau_x |D_q|^2)^{1/2} a\|_{L^2}$  and  $\|(1 + \tau_x |D_q|^2)^{1/2} \tilde{a}\|_{L^2}$  are uniformly equivalent because

$$e^{\pm i\frac{y}{2\sqrt{\tau_x}}} (\sqrt{\tau_x} D_y) e^{\mp i\frac{y}{2\sqrt{\tau_x}}} = (\sqrt{\tau_x} D_y) \mp \frac{1}{2}.$$

Hence it suffices to estimate  $\sqrt{\tau_x} \varepsilon D_q \hat{U}^* \psi$ . Remember that  $\hat{U} = U(q, \varepsilon D_q, \tau, \varepsilon)$  with  $U \in S_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , while  $\sqrt{\tau_x} p \in S_u(\langle \sqrt{\tau_x} p \rangle, g_\tau; \mathbb{R}^2)$ . With  $\|(1 + \tau_x |D_q|^2)^{1/2} \psi\|_{L^2} \leq C_{\ell_V,G}$  in Proposition 5.3, simply compute:

$$\sqrt{\tau_x} \varepsilon D_q \hat{U}^* \psi = \varepsilon \hat{U}^* \sqrt{\tau_x} D_q \psi + \left[ \sqrt{\tau_x} \varepsilon D_q, \hat{U}^* \right] \psi = \mathcal{O}(\varepsilon) \quad \text{in } L^2(\mathbb{R}^2; \mathbb{C}^2),$$

and divide by  $\varepsilon$  for (5.7).

In order to compare the energies, consider first the linear part by writing

$$\begin{aligned} \left| \langle \psi, H_{Lin} \psi \rangle - \varepsilon^{2+2\delta} \tau_x \left[ \langle a_+, \hat{H}_+ a_+ \rangle + \langle a_-, \hat{H}_- a_- \rangle \right] \right| = \\ \left| \langle \tilde{a}, (\hat{U}^* H_{Lin} \hat{U} - \varepsilon^{2+2\delta} H_{BO}) \tilde{a} \rangle \right|, \end{aligned}$$

with

$$\begin{aligned} \tilde{a} &= \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}, \\ H_{BO} &= \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} \hat{H}_+ e^{-i\frac{y}{2\sqrt{\tau_x}}} & 0 \\ 0 & e^{-i\frac{y}{2\sqrt{\tau_x}}} \hat{H}_- e^{i\frac{y}{2\sqrt{\tau_x}}} \end{pmatrix}, \\ \hat{H}_\pm &= -\partial_x^2 - (\partial_y \pm i \frac{x}{2\sqrt{1 + \tau_x x^2}})^2 + \frac{v(\sqrt{\tau_x \cdot})}{\ell_V^2 \tau_x} + \frac{(1 \pm 1)}{\varepsilon^{2+2\delta} \tau_x} (1 + \tau_x x^2)^{1/2}. \end{aligned}$$

Here it is convenient to write

$$\begin{aligned} \varepsilon^{2+2\delta} \tau_x H_{BO} &= \varepsilon^{2\delta} \hat{B} + \begin{pmatrix} 2(1 + \tau_x x^2)^{1/2} \\ 0 \end{pmatrix}, \\ \hat{B} &= \begin{pmatrix} \hat{B}_+ & 0 \\ 0 & \hat{B}_- \end{pmatrix}, \quad \hat{B}_\pm = B_\pm(q, \varepsilon D_q, \tau, \varepsilon), \end{aligned} \quad (5.11)$$

$$B_\pm(q, p, \tau, \varepsilon) = \tau_x p_x^2 + (\sqrt{\tau_x} p_y \pm \frac{\varepsilon}{2} (\frac{\sqrt{\tau_x} x}{\sqrt{1 + \tau_x x^2}} - \sqrt{\tau_x}))^2 + \frac{\varepsilon^2 v(\sqrt{\tau_x})}{\ell_V^2}. \quad (5.12)$$

With the notation  $\hat{\chi} = \chi(\tau_x \varepsilon^2 |D_q|^2)$  of Proposition 3.2, Lemma 5.5 below says in particular

$$\begin{aligned} \|(1 - \hat{\chi})\psi\|_{L^2}^2 &\leq C_{\ell_V, G} \left[ \langle \tilde{a}, \hat{B}\tilde{a} \rangle + \varepsilon^{1+2\delta} \|\tilde{a}\|_{L^2}^2 \right], \\ \|\sqrt{\tau_x} \varepsilon |D_q| (1 - \hat{\chi})\psi\|_{L^2}^2 &\leq C_{\ell_V, G} \left[ \langle \tilde{a}, \hat{B}\tilde{a} \rangle + \varepsilon^{1+2\delta} \|\tilde{a}\|_{L^2}^2 \right]. \end{aligned}$$

Proposition 3.2 yields

$$\left| \langle \tilde{a}, \left( \hat{U}^* H_{Lin} \hat{U} - \varepsilon^{2\delta} \hat{B} - \begin{pmatrix} 2(1 + \tau_x x^2)^{1/2} \\ 0 \end{pmatrix} \right) \tilde{a} \rangle \right| \leq C_{\ell_V, G} \left[ \varepsilon^{2+4\delta} + \varepsilon^{1+2\delta} \langle \tilde{a}, \hat{B}\tilde{a} \rangle \right].$$

For the nonlinear part of the energy, Proposition 3.3 gives

$$(1 - C\varepsilon^{1+2\delta}) \int_{\mathbb{R}^2} |\psi|^4 \leq \int_{\mathbb{R}^2} |\tilde{a}|^4 = \int_{\mathbb{R}^2} |a|^4 \leq (1 + C\varepsilon^{1+2\delta}) \int_{\mathbb{R}^2} |\psi|^4$$

with  $\tilde{a} = \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$  and  $a = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}$ . The bound  $\int_{\mathbb{R}^2} |\psi|^4 \leq C_{\ell_V, G} \tau_x^{-1}$

coming from  $\mathcal{E}_\varepsilon(\psi) = \mathcal{O}(\varepsilon^{2+2\delta})$  with  $\varepsilon^{2+2\delta} W_\tau = \mathcal{O}(\varepsilon^{2+2\delta})$ , leads to

$$\left| \frac{G\tau_x \varepsilon^{2+2\delta}}{2} \int_{\mathbb{R}^2} |\psi|^4 - \frac{G\tau_x \varepsilon^{2+2\delta}}{2} \int_{\mathbb{R}^2} |\tilde{a}|^4 \right| \leq C_{\ell_V, G} \varepsilon^{2+2\delta} \tau_x \times \varepsilon^{1+2\delta} \tau_x^{-1} = C_{\ell_V, G} \varepsilon^{3+4\delta},$$

which is smaller than the error term for the linear part. We have proved

$$\begin{aligned} \left| \mathcal{E}_\varepsilon(\psi) - \varepsilon^{2\delta} \langle \tilde{a}, \hat{B}\tilde{a} \rangle - \langle \tilde{a}_+, 2(1 + \tau_x x^2)^{1/2} \tilde{a}_+ \rangle - \frac{G_{\varepsilon, \tau}}{2} \int |a|^4 \right| \\ \leq C_{\ell_V, G} \left[ \varepsilon^{2+4\delta} + \varepsilon \times \varepsilon^{2\delta} \langle \tilde{a}, \hat{B}\tilde{a} \rangle \right]. \end{aligned}$$

With  $\mathcal{E}_\varepsilon(\psi) = \mathcal{E}_{\varepsilon, \min} (= \mathcal{O}(\varepsilon^{2+2\delta}))$ , this gives

$$(1 - C\varepsilon) \varepsilon^{2\delta} \langle \tilde{a}, \hat{B}\tilde{a} \rangle + 2 \langle \tilde{a}_+, (1 + \tau_x x^2)^{1/2} \tilde{a}_+ \rangle + \frac{G_{\varepsilon, \tau}}{2} \int |a|^4 \leq C\varepsilon^{2+4\delta} + \mathcal{E}_{\varepsilon, \min},$$

where all the terms of the left-hand side are now non negative. We deduce (5.8) and by bootstrapping

$$\begin{aligned} \varepsilon^{2+2\delta} \tau_x \langle a_-, \hat{H}_- a_- \rangle + \frac{G_{\varepsilon, \tau}}{2} \int |a|^4 &\leq \varepsilon^{2\delta} \langle \tilde{a}, \hat{B}\tilde{a} \rangle + \frac{G_{\varepsilon, \tau}}{2} \int |\tilde{a}|^4 \\ &\leq \mathcal{E}_{\varepsilon, \min} + C_{\ell_V, G} \varepsilon^{2+4\delta}. \end{aligned}$$

Additionally,  $\int |a|^4 = \int (|a_-|^2 + |a_+|^2)^2 \geq \int |a_-|^4$  also gives

$$0 \leq \|a_-\|_{L^2}^4 \mathcal{E}_{\tau, \min} \leq \mathcal{E}_{\tau}(a_-) \leq C_{\ell_V, G} \frac{\varepsilon^{2\delta}}{\tau_x} + \frac{\mathcal{E}_{\varepsilon, \min}}{\varepsilon^{2+2\delta} \tau_x} \leq \mathcal{E}_{\tau, \min} + C'_{\ell_V, G} \frac{\varepsilon^{2\delta}}{\tau_x}.$$

With  $\|a_-\|_{L^2}^2 = 1 - \|a_+\|^2 = 1 + \mathcal{O}(\varepsilon^{2+2\delta}) = 1 + \mathcal{O}(\frac{\varepsilon^{2\delta}}{\tau_x})$  and  $\mathcal{E}_{\tau, \min} = \mathcal{E}_{H, \min} + \mathcal{O}(\tau_x^{2/3})$ , this finally leads to

$$|\frac{\mathcal{E}_{\varepsilon, \min}}{\varepsilon^{2+2\delta} \tau_x} - \mathcal{E}_{\tau}(a_-)| \leq C''_{\ell_V, G} \frac{\varepsilon^{2\delta}}{\tau_x}.$$

□

**Lemma 5.5.** *Assume  $B(q, p, \tau, \varepsilon) = \tau_x |p|^2 + \varepsilon r$  with  $r \in S_u(\langle \sqrt{\tau_x} p \rangle, g_{\tau}; \mathcal{M}_2(\mathbb{C}))$ , take any  $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$  and set  $\hat{B} = B(q, \varepsilon D_q, \tau, \varepsilon)$  and  $\hat{\chi} = \chi(\tau_x \varepsilon |D_q|^2)$ . Then there exists  $\varepsilon_{B, \chi} > 0$  and  $C_{B, \chi} > 0$  such that the estimates*

$$\begin{aligned} \|(1 - \hat{\chi})u\|_{L^2}^2 + \|\sqrt{\tau_x} \varepsilon D_q (1 - \hat{\chi})u\|_{L^2}^2 &\leq C_{B, \chi} \left[ \langle u, \hat{B}u \rangle + \varepsilon^{1+2\delta} \|u\|_{L^2}^2 \right], \\ \text{and } \|(1 - \hat{\chi})u\|_{L^2} + \|\sqrt{\tau_x} \varepsilon D_q (1 - \hat{\chi})u\|_{L^2} &\leq C_{B, \chi} \left[ \|\hat{B}u\|_{L^2} + \varepsilon^{1+2\delta} \|u\|_{L^2} \right], \end{aligned}$$

hold uniformly w.r.t  $\delta \in (0, \delta_0]$  and  $\varepsilon \in (0, \varepsilon_{B, \chi})$ .

**Proof:** For  $\chi_0 \in \mathcal{C}_0^\infty(\mathbb{R})$  such that  $\chi_0 \geq 0$  and  $\chi_0 \equiv 1$  around 0, the symbol  $\chi_0(\tau_x p^2) + B$  is an elliptic symbol in  $S_u(\langle \sqrt{\tau_x} p \rangle^2, g_{\tau}; \mathcal{M}_2(\mathbb{C}))$ . For  $\varepsilon > 0$  small enough according to  $(\chi_0, B)$ , its quantization  $\hat{\chi}_0 + \hat{B}$  is invertible and its inverse belongs to  $OpS_u(\langle \sqrt{\tau_x} p \rangle^{-2}, g_{\tau}, \mathcal{M}_2(\mathbb{C}))$ . Next we notice that in

$$(1 - \hat{\chi}) = (1 - \hat{\chi}) \circ [\hat{\chi}_0 + \hat{B}]^{-1} \circ \hat{B} + (1 - \hat{\chi}) \circ [\hat{\chi}_0 + \hat{B}]^{-1} \circ \hat{\chi}_0,$$

the last term belongs to  $Op\mathcal{N}_{u, g_{\tau}}$  if  $\chi_0 \prec \chi$ . All the estimates are consequences of

$$(1 - \hat{\chi}) = (1 - \hat{\chi}) \circ [\hat{\chi}_0 + \hat{B}]^{-1} \circ \hat{B} + \varepsilon^{1+2\delta} \rho,$$

with  $\rho \in S_u(\frac{1}{\langle \tau_x p \rangle^\infty}, g_{\tau}; \mathcal{M}_2(\mathbb{C}))$ . □

## 5.4 Adiabatic Euler-Lagrange equation

As suggested by Proposition 4.7, or the last steps in the proof of Proposition 4.6, an accurate comparison of minimizers requires some comparison of the Euler-Lagrange equations. We check here that the  $a_-$  component in Proposition 5.4 solves approximately the Euler-Lagrange equations for minimizers of  $\mathcal{E}_{\tau}$ . Here the bootstrap argument is made in terms of operators instead of quadratic forms. In order to get reliable results, we now assume

$$\varepsilon^{2\delta} \leq c_{\ell_V, G} \tau_x,$$

with  $c_{\ell_V, G}$  chosen small enough.

With such an assumption we know:



- from (5.10) and  $|\mathcal{E}_{\tau,min} - \mathcal{E}_{H,min}| = \mathcal{O}(\tau_x^{2/3})$ ,

$$C^{-1}\varepsilon^{2+2\delta}\tau_x \leq \mathcal{E}_{\varepsilon,min} \leq C\varepsilon^{2+2\delta}\tau_x.$$

- When  $\psi \in \text{Argmin } \mathcal{E}_{\varepsilon,min}$  is written  $\psi = \hat{U} \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$  the  $L^4$ -norm of  $a$  is uniformly bounded,  $\int |a|^4 \leq C_{\ell_V,G}$ , according to (5.8). By applying Lemma 3.4 this also gives  $\int |\psi|^4 \leq C_{\ell_V,G}$ . We also have  $\|a_+\|_{L^2}^2 \leq C_{\ell_V,G}\varepsilon^{2+2\delta}\tau_x$ .
- The Lagrange multiplier  $\lambda_\psi$ , associated with  $\psi \in \text{Argmin } \mathcal{E}_{\varepsilon,min}$ , equals  $\mathcal{E}_\varepsilon(\psi) + \frac{G_{\varepsilon,\tau}}{2} \int |\psi|^4$ . Thus it is of order  $\mathcal{O}(\varepsilon^{2+2\delta}\tau_x)$ .

**Proposition 5.6.** *Under the same assumptions as in Proposition 5.4 and with the above condition  $\varepsilon^{2\delta} \leq c_{\ell_V,G}\tau_x$ , write a minimizer  $\psi$  of  $\mathcal{E}_\varepsilon$  in the form  $\psi =$*

$$\hat{U} \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}. \text{ Then the component } a_- \text{ solves the equation}$$

$$\hat{H}_- a_- + G \int |a_-|^2 a_- = \lambda_\psi a_- + r_\varepsilon \quad \text{with} \quad \|r_\varepsilon\|_{L^2} \leq C_{\ell_V,G}(\varepsilon + \frac{\varepsilon^{2\delta}}{\tau_x}),$$

while  $\|a_+\|_{L^2} \leq C_{\ell_V,G}\varepsilon^{2+2\delta}\tau_x$ .

The  $L^p$ -norms of  $a$  and  $\psi$  are uniformly bounded by  $C_{\ell_V,G}$  for  $p \in [2, 6]$ .

Moreover if  $\hat{B}$  is the operator defined in (5.11)-(5.12),  $\tilde{a} = \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$  satisfies

$$\|\hat{B}\tilde{a}\|_{L^2} \leq C_{\ell_V,G}\varepsilon^2\tau_x. \quad (5.13)$$

**Remark 5.7.** *The relation of  $\|\hat{B}\tilde{a}\|_{L^2}$  with  $\|\tilde{a}\|_{H^2}$  is given by*

$$C^{-1} [\varepsilon^2\tau_x \|D_q^2 \tilde{a}\| + \varepsilon^2 \|\tilde{a}\|_{L^2}] \leq \|\hat{B}\tilde{a}\|_{L^2} + \varepsilon^2 \|\tilde{a}\|_{L^2} \leq C [\varepsilon^2\tau_x \|D_q^2 \tilde{a}\| + \varepsilon^2 \|\tilde{a}\|_{L^2}].$$

Note that the  $L^2$  remainder terms have a factor  $\varepsilon^2$  and not  $\varepsilon^2\tau_x$ .

**Proof:** Playing with the Euler-Lagrange equation for  $\psi$ , we shall first prove (5.13) by using the same argument as we did for  $\langle \tilde{a}, \hat{B}\tilde{a} \rangle$  in the variational proof of Proposition 5.4 and then use it in order to estimate  $\|r\|_{L^2}$ . The Euler-Lagrange equation for  $\psi$

$$H_{Lin}\psi + G_{\varepsilon,\tau}|\psi|^2\psi = \lambda_\psi\psi$$

becomes

$$\hat{U}^* H_{Lin} \hat{U} \tilde{a} + G_{\varepsilon,\tau} \hat{U}^* (|\psi|^2 \psi) = \lambda_\psi \tilde{a}.$$

Remember that Born-Oppenheimer Hamiltonian is given by

$$\begin{aligned} \varepsilon^{2+2\delta}\tau_x H_{BO} &= \varepsilon^{2+2\delta}\tau_x \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} \hat{H}_+ e^{-i\frac{y}{2\sqrt{\tau_x}}} & 0 \\ 0 & e^{-i\frac{y}{2\sqrt{\tau_x}}} \hat{H}_- e^{i\frac{y}{2\sqrt{\tau_x}}} \end{pmatrix}, \\ &= \varepsilon^{2\delta} \hat{B} + \begin{pmatrix} 2\sqrt{1 + \tau_x x^2} \\ 0 \end{pmatrix}, \end{aligned}$$

by using the notations of (5.11)-(5.12).

Let us consider first the linear part after decomposing  $\tilde{a}$  into  $\tilde{a} = \hat{\chi}\tilde{a} + (1-\hat{\chi})\tilde{a}$ , where the kinetic energy cut-off operator  $\hat{\chi} = \chi(\tau_x|\varepsilon D_q|^2)$  has been introduced in Proposition 3.2:

$$\begin{aligned} \hat{U}^* H_{Lin} \hat{U} \tilde{a} &= \underbrace{\hat{U}^* H_{Lin} \hat{U} \hat{\chi} \tilde{a}}_{(I)} \\ &+ \underbrace{(\hat{U}^* - \hat{U}_0^*) H_{Lin} \hat{U} (1 - \hat{\chi}) \tilde{a} + \hat{U}_0^* H_{Lin} (\hat{U} - \hat{U}_0) (1 - \hat{\chi}) \tilde{a}}_{(II)} \\ &+ \underbrace{\hat{U}_0^* H_{Lin} \hat{U}_0 (1 - \hat{\chi}) \tilde{a}}_{(III)}. \end{aligned}$$

The three terms are treated by reconsidering the computations done for Proposition 3.2. By inserting a cut-off  $\hat{\chi}_1$ ,  $\chi \prec \chi_1$ , in  $\chi_1 \hat{U}^* H_{Lin} \hat{U} \hat{\chi} \tilde{a}$  with  $(1 - \hat{\chi}_1) \hat{U}^* H_{Lin} \hat{U} \hat{\chi} \in Op\mathcal{N}_{u, g_\tau}$ , we get

$$(I) = \varepsilon^{2+2\delta} \tau_x H_{BO} \hat{\chi} \tilde{a} + \mathcal{O}(\varepsilon^{2+4\delta}) \quad \text{in } L^2(\mathbb{R}^2).$$

With  $\varepsilon^{-1-2\delta}(\hat{U} - \hat{U}_0) \in OpS_u(\frac{1}{(\sqrt{\tau_x p})^\infty}, g_\tau; \mathcal{M}_2(\mathbb{C}))$  and by using Lemma 5.5, the second term is estimated by

$$\|(II)\|_{L^2} \leq C\varepsilon^{1+2\delta} \|(1 - \hat{\chi})\tilde{a}\|_{L^2} \leq C' \left[ \varepsilon \|\varepsilon^{2\delta} \hat{B} \tilde{a}\|_{L^2} + \varepsilon^{2+4\delta} \right].$$

We write the third term as

$$(III) = \varepsilon^{2+2\delta} \tau_x H_{BO} (1 - \hat{\chi}) \tilde{a} + \varepsilon^{2+2\delta} \tau_x \mathcal{D}_{kin} (1 - \hat{\chi}) \tilde{a} + \mathcal{D}_{pot} (1 - \hat{\chi}) \tilde{a},$$

where  $\mathcal{D}_{kin}$  and  $\mathcal{D}_{pot}$  are defined by (3.7)-(3.8). Following the arguments given in the proof of Proposition 3.2 after these definitions, we get

$$\begin{aligned} \|\mathcal{D}_{pot} (1 - \hat{\chi}) \tilde{a}\|_{L^2} &\leq C\varepsilon^{1+2\delta} \|(1 - \hat{\chi})\tilde{a}\|_{L^2} \leq \\ &\leq C' \left[ \varepsilon \|\varepsilon^{2\delta} \hat{B} \tilde{a}\|_{L^2} + \varepsilon^{2+4\delta} \right], \\ \|\mathcal{D}_{kin} (1 - \hat{\chi}) \tilde{a}\|_{L^2} &\leq C \left[ \varepsilon^{1+4\delta} \|(1 - \hat{\chi})\tilde{a}\|_{L^2} + \varepsilon^{1+2\delta} \|(\varepsilon \sqrt{\tau_x} |D_q|) (1 - \hat{\chi}) \tilde{a}\|_{L^2} \right] \\ &\leq C' \left[ \varepsilon \|\varepsilon^{2\delta} \hat{B} \tilde{a}\|_{L^2} + \varepsilon^{2+4\delta} \right]. \end{aligned}$$

Hence the Euler-Lagrange equation can be written

$$\begin{aligned} \varepsilon^{2+2\delta} \tau_x H_{BO} \tilde{a} &= \lambda_\psi \tilde{a} - \varepsilon^{2+2\delta} \tau_x G \hat{U}^* (|\psi|^2 \psi) + r \\ \text{with } \|r\|_{L^2} &\leq C \left[ \varepsilon \|\varepsilon^{2\delta} \hat{B} \tilde{a}\|_{L^2} + \varepsilon^{2+4\delta} \right]. \end{aligned}$$

From Proposition 5.3, with  $\varepsilon^{2\delta} \leq c\tau_x$ , we know  $\|\psi\|_{L^4} \leq C$ . It can be transformed into  $\|\tilde{a}\|_{L^4} = \|\hat{U}^* \psi\|_{L^4} \leq C$  with

$$\| |\psi|^2 \psi \|_{L^2} \leq C \|\psi\|_{L^6}^3 \leq C' \|\tilde{a}\|_{L^6}^3,$$

by applying Lemma 3.4, adapted for the metric  $g_\tau$  like in the proof Proposition 3.3. We start from the interpolation inequality

$$\|f\|_{L^6} \leq C \|D_q^2 f\|_{L^2}^{\frac{1}{9}} \|f\|_{L^4}^{\frac{8}{9}} \leq \frac{C}{(\tau_x \varepsilon)^{\frac{2}{9}}} \|\tau_x^2 \varepsilon^2 D_q^2 f\|_{L^2}^{\frac{1}{9}} \|f\|_{L^4}^{\frac{8}{9}}.$$

By introducing the operator  $\tilde{B} = B(\tau_x^{-1/2} \varepsilon q, \tau_x^{\frac{1}{2}} D_q, \tau, \varepsilon)$  with

$$\begin{aligned} B_\pm(\tau_x^{-1/2} q, \tau_x^{1/2} D_q, \tau, \varepsilon) &= (\tau_x \varepsilon)^2 D_q^2 \pm \frac{\varepsilon}{2} \left( \frac{x}{\sqrt{1+x^2}} - \sqrt{\tau_x} \right) (\tau_x \varepsilon) D_y \\ &\quad + \frac{\varepsilon^2}{4} \left[ \left( \frac{x}{\sqrt{1+x^2}} - \sqrt{\tau_x} \right)^2 + \frac{4v}{\ell_V^2} \right], \end{aligned}$$

it becomes

$$\|f\|_{L^6} \leq \frac{C_{\ell_V}}{(\tau_x \varepsilon)^{\frac{2}{9}}} \left[ \|\tilde{B}f\|_{L^2}^{\frac{1}{9}} \|f\|_{L^4}^{\frac{8}{9}} + \varepsilon^{\frac{2}{9}} \|f\|_{L^2}^{\frac{1}{9}} \|f\|_{L^4}^{\frac{8}{9}} \right].$$

The above relation with  $f = \tau_x^{-\frac{1}{2}} \tilde{a}(\tau_x^{-\frac{1}{2}} \cdot)$  which satisfies

$$\|f\|_{L^6} = \tau_x^{-\frac{1}{3}} \|\tilde{a}\|_{L^6}, \quad \|f\|_{L^4} = \tau_x^{-\frac{1}{2}} \|\tilde{a}\|_{L^4} \quad \text{and} \quad \|\tilde{B}f\|_{L^2} = \|\hat{B}\tilde{a}\|_{L^2}$$

leads to

$$\begin{aligned} \tau_x^{-\frac{1}{3}} \|\tilde{a}\|_{L^6} &\leq \frac{C_{\ell_V}}{(\tau_x \varepsilon)^{\frac{2}{9}}} \left[ \|\hat{B}\tilde{a}\|_{L^2}^{\frac{1}{9}} \tau_x^{-\frac{4}{9}} \|\tilde{a}\|_{L^4}^{\frac{8}{9}} + \varepsilon^{\frac{2}{9}} \|\tilde{a}\|_{L^2}^{\frac{1}{9}} \tau_x^{-\frac{4}{9}} \|\tilde{a}\|_{L^4}^{\frac{8}{9}} \right] \\ &\leq C_{\ell_V, G} \tau_x^{-\frac{1}{3}} \left[ \varepsilon^{-\frac{2}{9}} \|\hat{B}\tilde{a}\|_{L^2}^{\frac{1}{9}} + 1 \right], \end{aligned}$$

and finally

$$G_{\varepsilon, \tau} \| |\psi|^2 \psi \|_{L^2} \leq G \varepsilon^{2+2\delta} \tau_x \|\psi\|_{L^6}^3 \leq C_{\ell_V, G} \left[ \varepsilon^{4/3} \tau_x \|\varepsilon^{2\delta} \hat{B}\tilde{a}\|_{L^2} + \varepsilon^{2+2\delta} \tau_x \right]$$

With  $|\lambda_\psi| = \mathcal{O}(\varepsilon^{2+2\delta} \tau_x)$ , we obtain

$$\|\varepsilon^{2+2\delta} \tau_x H_{BO} \tilde{a}\|_{L^2} \leq C \left[ \varepsilon \|\varepsilon^{2\delta} \hat{B}\tilde{a}\|_{L^2} + \varepsilon^{2+4\delta} + \varepsilon^{2+2\delta} \tau_x \right],$$

and recall

$$\varepsilon^{2+2\delta} \tau_x H_{BO} = \begin{pmatrix} \varepsilon^{2\delta} \hat{B}_+ + 2\sqrt{1 + \tau_x x^2} \\ \varepsilon^{2\delta} \hat{B}_- \end{pmatrix}.$$

According to Lemma 5.8 below

$$\|\varepsilon^{2\delta} \hat{B}_+ \tilde{a}_+\|_{L^2} + \|2\sqrt{1 + \tau_x x^2} \tilde{a}_+\|_{L^2} \leq C \|\varepsilon^{2\delta} \hat{B}_+ + 2\sqrt{1 + \tau_x x^2}\| \tilde{a}_+\|_{L^2}.$$

We deduce

$$\|\varepsilon^{2\delta} \hat{B}\tilde{a}\|_{L^2} \leq C \varepsilon^{2+2\delta} \tau_x.$$

Plugging this result into the estimate of the remainder  $r$  gives

$$\varepsilon^{2+2\delta}\tau_x H_{BO}\tilde{a} = \lambda_\tau \tilde{a} + G_{\varepsilon,\tau}\hat{U}^*(|\psi|^2\psi) + \mathcal{O}(\varepsilon^{3+2\delta}\tau_x + \varepsilon^{2+4\delta}).$$

Consider now more carefully the nonlinear term

$$\begin{aligned} \hat{U}^*(|\psi|^2\psi) &= \underbrace{\hat{U}_0^* \left[ |\hat{U}_0\tilde{a}|^2(\hat{U}_0\tilde{a}) \right]}_{(1)} + \underbrace{(\hat{U}^* - \hat{U}_0^*) \left[ |\hat{U}_0\tilde{a}|^2(\hat{U}_0\tilde{a}) \right]}_{(2)} \\ &\quad + \underbrace{\hat{U}^* \left[ |\hat{U}\tilde{a}|^2(\hat{U}\tilde{a}) - |\hat{U}_0\tilde{a}|^2(\hat{U}_0\tilde{a}) \right]}_{(3)}. \end{aligned}$$

By differentiating the relation  $\int |f|^4 = \int |\hat{U}_0 f|^4$  w.r.t  $f$ , the first term equals

$$(1) = |\tilde{a}|^4 \tilde{a}.$$

By semiclassical calculus in the metric  $g_\tau$ , the operator  $\sqrt{\tau_x}\varepsilon D_q \hat{U}_0$  equals

$$\sqrt{\tau_x}\varepsilon D_q \hat{U}_0 = \hat{U}_0 \sqrt{\tau_x}\varepsilon D_q + \left[ \sqrt{\tau_x}\varepsilon D_q, \hat{U}_0 \right] \psi = \hat{U}_0 \sqrt{\tau_x}\varepsilon D_q + \mathcal{O}(\varepsilon),$$

where the remainder estimate holds in  $\mathcal{L}(L^2(\mathbb{R}^2; \mathbb{C}^2))$ . We have already proved  $\|\tilde{a}\|_{L^6} \leq C$  and Lemma 3.4 leads again to

$$\|\hat{U}\tilde{a}\|_{L^6} + \|\hat{U}_0\tilde{a}\|_{L^6} \leq C.$$

With  $\varepsilon^{-1-2\delta}(\hat{U} - \hat{U}_0) \in OpS_u(1, g_\tau; \mathcal{M}_2(\mathbb{C}))$ , this gives

$$\|(2)\| \leq C\varepsilon^{1+2\delta}.$$

For the third term, we use

$$\begin{aligned} \left\| \left[ |\hat{U}\tilde{a}|^2(\hat{U}\tilde{a}) - |\hat{U}_0\tilde{a}|^2(\hat{U}_0\tilde{a}) \right] \right\|_{L^2} &\leq C_0 \|(\hat{U} - \hat{U}_0)\tilde{a}\|_{L^6} \left[ \|\hat{U}\tilde{a}\|_{L^6}^2 + \|\hat{U}_0\tilde{a}\|_{L^6}^2 \right] \\ &\leq C\varepsilon^{1+2\delta}. \end{aligned}$$

We have proved

$$G_{\tau,\varepsilon}\hat{U}^*(|\psi|^2\psi) - G_{\tau,\varepsilon}|\tilde{a}|^2\tilde{a} = \mathcal{O}(\varepsilon^{3+4\delta}\tau_x),$$

which is even better than the estimate for the linear part.

For the  $\tilde{a}_-$  component, we get

$$H_{BO} \begin{pmatrix} 0 \\ \tilde{a}_- \end{pmatrix} + G(|\tilde{a}_-|^2 + |\tilde{a}_+|^2)\tilde{a}_- = \frac{\lambda_\psi}{\varepsilon^{2+2\delta}\tau_x}\tilde{a}_- + \mathcal{O}(\varepsilon + \frac{\varepsilon^{2\delta}}{\tau_x}),$$

and it remains to estimate the term  $|\tilde{a}_+|^2\tilde{a}_-$ . The first line of the system may be written

$$\varepsilon^{2\delta}\hat{B}_+\tilde{a}_+ + 2\sqrt{1+\tau_x x^2}\tilde{a}_+ + G_{\varepsilon,\tau}(|\tilde{a}_+|^2 + |\tilde{a}_-|^2)\tilde{a}_+ = \lambda_\psi\tilde{a}_+ + \mathcal{O}(\varepsilon^{3+2\delta}\tau_x + \varepsilon^{2+2\delta}\tau_x).$$

Taking the scalar product with  $\tilde{a}_+$ , with  $\lambda_\tau = \mathcal{O}(\varepsilon^{2+2\delta}\tau_x)$  and  $\hat{B}_+ \geq 0$ , gives

$$\int |\tilde{a}_+|^4 \leq C[\|\tilde{a}_+\|_{L^2}^2 + (\varepsilon + \frac{\varepsilon^{2\delta}}{\tau_x})\|a_+\|_{L^2}] \leq C'\varepsilon^{2+2\delta}\tau_x.$$

Then the same argument as in the estimate of  $\|\tilde{a}\|_{L^6}$  gives

$$\begin{aligned} \|\tilde{a}_+\|_{L^6} &\leq C \left[ \varepsilon^{-\frac{2}{9}} \|\hat{B}_+ \tilde{a}_+\|_{L^2}^{\frac{1}{9}} \|\tilde{a}_+\|_{L^4}^{\frac{8}{9}} + \|\tilde{a}_+\|_{L^2}^{\frac{1}{9}} \|\tilde{a}_+\|_{L^4}^{\frac{8}{9}} \right] \\ &\leq C' \left[ (\varepsilon^{-2-2\delta} \|\varepsilon^{2\delta} \hat{B}_+ \tilde{a}_+\|_{L^2})^{\frac{1}{9}} + (\varepsilon^{2+2\delta} \tau_x)^{\frac{1}{18}} \right] (\varepsilon^{2+2\delta} \tau_x)^{\frac{2}{9}} \\ &\leq C'' \tau_x^{\frac{1}{9}} (\varepsilon^{2+2\delta} \tau_x)^{\frac{2}{9}} \leq C'' \varepsilon^{\frac{4+4\delta}{9}} \tau_x^{\frac{1}{3}}. \end{aligned}$$

Again with  $\|\tilde{a}\|_{L^6} \leq C$ , we deduce

$$\| |\tilde{a}_+|^2 \tilde{a}_- \|_{L^2} \leq C_{\ell_V, G} \varepsilon^{\frac{8+8\delta}{3}} \tau_x^{\frac{2}{3}} \leq C'_{\ell_V, G} \varepsilon.$$

The final result is just a transcription in terms of  $a$ . □

**Lemma 5.8.** *Let  $B_+$  be the symbol*

$$B_+(q, p, \tau_x, \varepsilon) = \tau_x p_x^2 + (\sqrt{\tau_x} p_y + \frac{\varepsilon}{2} (\frac{\sqrt{\tau_x} x}{\sqrt{1 + \tau_x x^2}} - \sqrt{\tau_x}))^2 + \frac{\varepsilon^2 v(\sqrt{\tau_x} \cdot)}{\ell_V^2}$$

introduced in (5.12). By setting  $\hat{B}_+ = B_+(q, \varepsilon D_q, \tau_x, \varepsilon)$ , the operator  $A = \varepsilon^{2\delta} \hat{B}_+ + 2\sqrt{1 + \tau_x x^2}$  is self-adjoint with  $D(A) = \{u \in L^2(\mathbb{R}^2), Au \in L^2(\mathbb{R}^2)\}$  as soon as  $\varepsilon \leq \varepsilon_0$ , with  $\varepsilon_0$  independent of  $\tau_x$ . Moreover the inequality

$$\forall u \in D(A), \quad \|\varepsilon^{2\delta} \hat{B}_+ u\|_{L^2} + \|2\sqrt{1 + \tau_x x^2} u\|_{L^2} \leq C \|Au\|_{L^2}$$

holds with a constant  $C$  independent of  $(\varepsilon, \tau_x)$ .

**Proof:** The operator  $A$  can be written

$$A = a_0(q, \varepsilon^{1+\delta} D_q, \tau_x) + \varepsilon^{1+\delta} a_1(q, \varepsilon^{1+\delta} D_q, \tau_x) + \varepsilon^{2+2\delta} a_2(q, \tau_x),$$

with  $a_k \in S_u(\langle \sqrt{\tau_x} p \rangle^{2-k} + \langle \sqrt{\tau_x} x \rangle^{(1-k)_+}, g_\tau)$  and

$$a_0(q, p, \tau_x) = p^2 + 2\sqrt{1 + \tau_x x^2}.$$

Therefore the operator  $A$  is elliptic in  $OpS_u(\langle \sqrt{\tau_x} p \rangle^2 + \langle \sqrt{\tau_x} x \rangle, g_\tau)$  and the result about the domain follows with

$$\|\varepsilon^{2\delta} \hat{B}_+ u\|_{L^2} + \|2\sqrt{1 + \tau_x x^2} u\|_{L^2} \leq C(\|Au\|_{L^2} + \|u\|_{L^2})$$

for all  $u \in D(A)$ . We conclude with

$$2\|u\|_{L^2}^2 \leq \langle u, Au \rangle \leq \|u\|_{L^2} \|Au\|_{L^2}$$

due to  $\hat{B}_+ \geq 0$ . □

## 5.5 End of the proof of Theorem 1.2

Assume  $G, \ell_V > 0$  be fixed and  $\delta \in (0, \delta_0]$ . Although we dropped  $\delta_0$  in our notations, all the constants in the previous inequalities depend on  $(G, \ell_V, \delta_0)$ . We assume now  $\tau_x \leq \tau_{\ell_V, G, \delta_0}$ ,  $\varepsilon \leq \varepsilon_{\ell_V, G, \delta_0}$  and

$$\varepsilon^{2\delta} \leq \tau_x^{\frac{5}{3}}.$$

Proposition 5.4 says

$$|\mathcal{E}_{\varepsilon, \min} - \varepsilon^{2+2\delta} \tau_x \mathcal{E}_{\tau, \min}| \leq C \varepsilon^{2+4\delta} \leq C' \varepsilon^{2+2\delta} \tau_x^{\frac{5}{3}}$$

and we recall

$$|\mathcal{E}_{\tau, \min} - \mathcal{E}_{H, \min}| \leq C \tau_x^{\frac{2}{3}}$$

by Proposition 4.6.

When  $\psi = \hat{U} \begin{pmatrix} e^{i\frac{y}{2\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{2\sqrt{\tau_x}}} a_- \end{pmatrix}$ , Proposition 5.6 says

$$\|a_+\|_{L^2} \leq C \varepsilon^{2+2\delta} \tau_x, \quad \|a\|_{H^2} \leq \frac{C}{\tau_x} \quad \text{and} \quad \|a\|_{L^4} + \|a\|_{L^6} \leq C,$$

while  $a_-$  solves the approximate Euler-Lagrange equation

$$\hat{H}_- a_- + G \int |a_-|^2 a_- = \lambda_\psi a_- + r_\varepsilon \quad \text{with} \quad \|r_\varepsilon\|_{L^2} \leq C_{\ell_V, G} \left( \varepsilon + \frac{\varepsilon^{2\delta}}{\tau_x} \right).$$

For  $u = \|a_-\|_{L^2}^{-1} a_-$  the energy  $\mathcal{E}_\tau(u)$  satisfy

$$|\mathcal{E}_\tau(u) - \mathcal{E}_{\tau, \min}| \leq C \tau_x^{\frac{2}{3}}$$

and the above equation becomes

$$\hat{H}_- u + G \int |u|^2 u = \lambda_\psi u + \mathcal{O}\left(\varepsilon + \frac{\varepsilon^{2\delta}}{\tau_x}\right).$$

We conclude by referring to Proposition 4.7 applied to  $u$  and then renormalizing for  $a_-$ : For  $\chi = (\chi_1, \chi_2)$  with  $\chi_1 \in \mathcal{C}_0^\infty(\mathbb{R}^2)$ ,  $\chi_1^2 + \chi_2^2 \equiv 1$ ,  $\chi_1 = 1$  in a neighborhood of 0

$$\begin{aligned} \|\chi_2(\tau_x^{\frac{1}{9}} \cdot) a_-\|_{L^2} &\leq C \tau_x^{\frac{1}{3}} \\ |\mathcal{E}_\tau(\chi_1(\tau_x^{\frac{1}{9}} \cdot) a_-) - \mathcal{E}_{H, \min}| &\leq C \tau_x^{\frac{2}{3}} \\ d_{\mathcal{H}_2}(\chi_1(\tau_x^{\frac{1}{9}} \cdot) a_-, \text{Argmin } \mathcal{E}_H) &\leq C \left( \tau_x^{\frac{2\nu_{\ell_V, G}}{3}} + \varepsilon \right), \quad \nu_{\ell_V, G} \in (0, \frac{1}{2}]. \end{aligned}$$

For the  $L^\infty$ -estimates of  $a_+$  and  $d_{L^\infty}(\chi_1(\tau_x^{\frac{1}{9}} \cdot) a_-, \text{Argmin } \mathcal{E}_H)$ , we simply use the interpolation inequality

$$\|u\|_{L^\infty} \leq C \|u\|_{L^2}^{\frac{1}{2}} \|\Delta u\|_{L^2}^{\frac{1}{2}} \leq C \|u\|_{L^2}^{\frac{1}{2}} \|u\|_{H^2}^{\frac{1}{2}},$$

valid for any  $u \in H^2(\mathbb{R}^2)$  (write  $u(0) = \int_{\mathbb{R}^2} \hat{u}(\xi) \frac{d\xi}{(2\pi)^2}$ , cut the integral according to  $|\xi| \leq R$ , estimate both term by Cauchy-Schwartz with  $\hat{u} = \frac{1}{|\xi|^2} (|\xi|^2 \hat{u})$  when  $|\xi| \geq R$ , and then optimize w.r.t  $R$ ).

## 6 Additional comments

We briefly discuss and sketch how our analysis could be adapted to other problems. No definite statement is given. Complete proofs require additional work, which may be done in the future.

### 6.1 About the smallness condition of $\varepsilon$ w.r.t $\tau_x$

In our main result, Theorem 1.2, condition (1.18) is used, namely

$$\varepsilon^{2\delta} \leq \frac{\tau_x^{\frac{5}{3}}}{C_\delta}.$$

One may wonder whether such a condition is necessary in order to compare the minimization problems for  $\mathcal{E}_\varepsilon$  and  $\varepsilon^{2+2\delta}\tau_x\mathcal{E}_H$ . When comparing the minimal energies in Proposition 5.4, we found

$$|\mathcal{E}_{\varepsilon,min} - \varepsilon^{2+2\delta}\mathcal{E}_{H,min}| \leq C\varepsilon^{2+4\delta},$$

while we know that  $\mathcal{E}_{H,min} = \mathcal{E}_{H,min}(\ell_V, G)$  is a positive number independent of  $\tau_x$  and  $\varepsilon$ . Hence it seems natural to say that  $\varepsilon^{2\delta} \ll \tau_x$ , at least, is required to ensure that  $\varepsilon^{2+2\delta}\tau_x\mathcal{E}_{H,min}$  is a good approximation of  $\mathcal{E}_{\varepsilon,min}$ . The error is made of three parts:

- the error term for the Born-Oppenheimer approximation in the low-frequency range given in Theorem 2.1;
- the error term coming from the truncated high frequency part;
- the non linear term.

The non linear term is  $\frac{G\varepsilon^{2+2\delta}\tau_x}{2} \int |\psi|^4$ , so that a small error in  $\|\psi\|_{L^4}^4$  will give a negligible term w.r.t  $\varepsilon^{2+2\delta}\tau_x\mathcal{E}_{H,min}$ . The question is thus mainly about the linear problem. If one looks more carefully at the error term of Theorem 2.1, it is made of the term

$$-\varepsilon^2 \frac{(\partial_{p_k} f_\varepsilon)(\partial_{p_\ell} f_\varepsilon)}{E_+ - E_-} \overline{X}_k X_\ell, \quad (6.1)$$

according to Proposition 2.6, and of terms coming from the third order term of Moyal products. The function  $f_\varepsilon$  is in our case  $f_\varepsilon(p) = \varepsilon^{2\delta}\tau_x p^2 \gamma(\tau_x p^2)$ ,  $p = (p_x, p_y)$ ,  $k, \ell \in \{x, y\}$ , and the factors  $X_x$  and  $X_y$  computed in the proof of Proposition 3.1 are at most of order  $\frac{1}{\sqrt{\tau_x}}$ . Hence the quantity (6.1) is an  $\mathcal{O}(\varepsilon^{2+4\delta}\tau_x)$  which is again negligible w.r.t  $\varepsilon^{2+2\delta}\tau_x\mathcal{E}_{H,min}$ . By considering the higher order terms in the Moyal product, the fast oscillating part of the symbol w.r.t  $y$ , at the frequency  $\frac{1}{\sqrt{\tau_x}}$ , deteriorates the estimates: although there are compensations with the slow variations w.r.t  $p_y$ , always multiplied by  $\sqrt{\tau_x}$ , only an  $\varepsilon^k$  factor without  $\tau_x$  appears in the  $k$ -th order term.

Hence, computing the higher order terms, at least up to order 3, in the adiabatic approximation and then considering the question of the high-frequency truncation, is a way to understand whether the smallness of  $\varepsilon$  w.r.t  $\tau_x$  is necessary.

## 6.2 Anisotropic nonlinearity

Our work assumes an isotropic nonlinearity. A more general nonlinear term would be

$$\frac{G\varepsilon^{2+2\delta}\tau_x}{2} \int \alpha_1 |\psi_1|^4 + 2\alpha_{12} |\psi_1|^2 |\psi_2|^2 + \alpha_2 |\psi_2|^4 \, dxdy, \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}.$$

Our case is  $\alpha_1 = \alpha_2 = \alpha_{12} = 1$ . Let  $\psi = \hat{U}\phi$ , with the unitary transform  $\hat{U} = \hat{U}_0 + \varepsilon^{1+2\delta}\hat{R}$ , (or conversely  $\phi = \hat{U}^*\psi$ ). Then the same arguments as in Subsection 3.3 will lead to

$$\begin{aligned} & \int \alpha_1 |\psi_1|^4 + 2\alpha_{12} |\psi_1|^2 |\psi_2|^2 + \alpha_2 |\psi_2|^4 \, dxdy \\ &= \left( \int \alpha_1 |\psi_1^0|^4 + 2\alpha_{12} |\psi_1^0|^2 |\psi_2^0|^2 + \alpha_2 |\psi_2^0|^4 \, dxdy \right) (1 + \mathcal{O}(\varepsilon^{1+2\delta})), \end{aligned}$$

after setting  $\psi^0(q) = u_0(q)\phi(q)$  at every  $q = (x, y)$ . In our case

$$u_0(x, y) = \begin{pmatrix} C & Se^{i\varphi} \\ Se^{-i\varphi} & -C \end{pmatrix}, \quad C = \cos\left(\frac{\theta}{2}\right), \quad S = \sin\left(\frac{\theta}{2}\right),$$

with  $\theta = \underline{\theta}(\sqrt{\tau_x}x)$ ,  $\varphi = \frac{y}{\sqrt{\tau_x}}$ . The point-wise identities

$$\begin{aligned} |\psi_1^0|^2 + |\psi_2^0|^2 &= |\phi_1|^2 + |\phi_2|^2 \\ |\psi_1^0|^2 - |\psi_2^0|^2 &= \cos(\theta) (|\phi_1|^2 - |\phi_2|^2) + 2\sin(\theta) \operatorname{Re}(\overline{\phi_1 e^{i\varphi}} \phi_2), \end{aligned}$$

lead to

$$\begin{aligned} \alpha_1 |\psi_1^0|^4 + 2\alpha_{12} |\psi_1^0|^2 |\psi_2^0|^2 + \alpha_2 |\psi_2^0|^4 &= \frac{\alpha_1 + 2\alpha_{12} + \alpha_2}{4} (|\phi_1|^2 + |\phi_2|^2)^2 \\ &+ \frac{\alpha_1 - \alpha_2}{2} (|\phi_1|^2 + |\phi_2|^2) \left( \cos(\theta) (|\phi_1|^2 - |\phi_2|^2) + 2\sin(\theta) \operatorname{Re}(\overline{\phi_1 e^{i\varphi}} \phi_2) \right) \\ &+ \frac{\alpha_1 - 2\alpha_{12} + \alpha_2}{4} \left( \cos(\theta) (|\phi_1|^2 - |\phi_2|^2) + 2\sin(\theta) \operatorname{Re}(\overline{\phi_1 e^{i\varphi}} \phi_2) \right)^2 \\ &= \left[ \alpha_1 \cos^4\left(\frac{\theta}{2}\right) + \alpha_2 \sin^4\left(\frac{\theta}{2}\right) + \frac{\alpha_{12}}{2} \sin^2(\theta) \right] |\phi_1|^4 \\ &+ \left[ \alpha_1 \sin^4\left(\frac{\theta}{2}\right) + \alpha_2 \cos^4\left(\frac{\theta}{2}\right) + \frac{\alpha_{12}}{2} \sin^2(\theta) \right] |\phi_2|^4 \\ &+ \left[ \frac{(\alpha_1 + \alpha_2)}{2} \sin^2(\theta) + \alpha_{12}(1 + \cos^2(\theta)) \right] |\phi_1|^2 |\phi_2|^2 \\ &+ [(\alpha_1 - \alpha_2) + (\alpha_1 - 2\alpha_{12} + \alpha_2) \cos(\theta)] \sin(\theta) |\phi_1|^2 \operatorname{Re}(\overline{\phi_1 e^{i\varphi}} \phi_2) \\ &+ [(\alpha_1 - \alpha_2) - (\alpha_1 - 2\alpha_{12} + \alpha_2) \cos(\theta)] \sin(\theta) |\phi_2|^2 \operatorname{Re}(\overline{\phi_1 e^{i\varphi}} \phi_2) \\ &+ (\alpha_1 - 2\alpha_{12} + \alpha_2) \sin^2(\theta) \operatorname{Re} \left[ \overline{(\phi_2 e^{i\varphi})} \phi_2 \right]. \end{aligned}$$

At least three points have to be adapted from the previous analysis:



- 1) When we take a test function  $\psi = \hat{U} \begin{pmatrix} 0 \\ e^{-i\frac{y}{\sqrt{\tau_x}}} a_- \end{pmatrix}$  the energy  $\mathcal{E}_\varepsilon(\psi)$  will be close to  $\varepsilon^{2+2\delta} \tau_x \mathcal{E}_\tau(a_-)$ , with

$$\begin{aligned} \mathcal{E}_\tau(a_-) &= \langle a_- , \hat{H}_- a_- \rangle \\ &+ \frac{G}{2} \int \left[ \alpha_1 \cos^4\left(\frac{\theta}{2}\right) + \alpha_2 \sin^4\left(\frac{\theta}{2}\right) + \frac{\alpha_{12}}{2} \sin^2(\theta) \right] |a_-|^4 \, dx dy, \end{aligned}$$

and  $\cos(\theta) = \frac{\sqrt{\tau_x x}}{\sqrt{1+\tau_x x^2}}$ . Hence before taking the limit  $\tau_x \rightarrow 0$  we have a position dependent nonlinearity. This will induce another error term when comparing with the energy  $\mathcal{E}_H(a_-) = \langle a_- , H_{\ell_V} a_- \rangle + \frac{G(\alpha_1 + \alpha_2 + 2\alpha_{12})}{8} \int |a_-|^4$ , in the limit  $\tau_x \rightarrow 0$ .

Another possibility consists in considering the case when  $|\alpha_2 - \alpha_1| + |\alpha_{12} - \alpha_1|$  is small as  $(\varepsilon, \tau_x) \rightarrow (0, 0)$ . The energy  $\mathcal{E}_\tau(\psi)$ , written as,

$$\begin{aligned} &\langle a_- , \hat{H}_- a_- \rangle \\ &+ \frac{G}{2} \int \left[ \alpha_1 + (\alpha_2 - \alpha_1) \sin^4\left(\frac{\theta}{2}\right) + \frac{(\alpha_{12} - \alpha_1)}{2} \sin^2(\theta) \right] |a_-|^4 \, dx dy, \end{aligned}$$

will converge to  $\mathcal{E}_H(a_-) = \langle a_- , H_{\ell_V} a_- \rangle + \frac{G\alpha_1}{2} \int |a_-|^4$ .

- 2) The existence of a minimizer for  $\mathcal{E}_\varepsilon$  and the variational argument showing that  $\|a_+\|_{L^2}^2 = \mathcal{O}(\varepsilon^{2+4\delta}) + \mathcal{E}_{\varepsilon, \min}$  when  $\psi = \hat{U} \begin{pmatrix} e^{i\frac{y}{\sqrt{\tau_x}}} a_+ \\ e^{-i\frac{y}{\sqrt{\tau_x}}} a_- \end{pmatrix}$  is a ground state for  $\mathcal{E}_\varepsilon$  will be essentially the same as in the isotropic case.
- 3) The analysis and the use of the Euler-Lagrange equation for ground states of  $\mathcal{E}_\varepsilon$ , like in Subsection 5.4, will certainly be more delicate because it will be a system, and the vanishing of the crossing terms have to be considered more carefully.

### 6.3 Minimization for excited states

One may consider like in [DGJO] the question of minimizing the energy, for states prepared according to  $\psi_+$  local eigenvector of the potential. Two things have to be modified in order to adapt the previous analysis:

- 1) The space of states, on which the energy is minimized has to be specified. The unitary transform  $\hat{U}$  introduced in Theorem 2.1 provides a simple way to formulate this minimization problem: set  $\mathcal{F}_+ = \text{Ran } \hat{U} P_+$  with  $P_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$  and consider

$$\inf_{\psi \in \mathcal{F}_+, \|\psi\|=1} \mathcal{E}_\varepsilon(\psi).$$

- 2) In order to get asymptotically as  $\varepsilon \rightarrow 0$ , the same scalar minimization problems with  $\mathcal{E}_\tau$  and  $\mathcal{E}_H$ , the external potential  $V_{\varepsilon,\tau}$  has to be changed. It must be now

$$V_{\varepsilon,\tau}(x, y) = \frac{\varepsilon^{2+2\delta}}{\ell_V^2} v(\sqrt{\tau_x}x, \sqrt{\tau_x}y) - \sqrt{1 + \tau_x x^2} - \varepsilon^{2+2\delta} \left[ \frac{\tau_x^2}{(1 + \tau_x x^2)^2} + \frac{1}{1 + \tau_x x^2} \right].$$

The analysis of this problem is essentially the same as for the complete minimization problem. It is even simpler because the unitary  $\hat{U}$  is directly introduced. A slightly different question is about the minimization of the energy  $\mathcal{E}_\varepsilon$  in the space  $\mathcal{F}_+^0 = \text{Ran } \hat{U}_0 P_+$ , but the accurate comparison between  $\hat{U}$  and  $\hat{U}_0$  widely used through this article would lead to similar results.

Possibly this extension can even be generalized to higher rank matricial potentials with eigenvectors  $\psi_1, \dots, \psi_N$ , for states modeled on any given  $\psi_k$ .

#### 6.4 Time dynamics of adiabatically prepared states

Nonlinear adiabatic time evolution has been considered recently in [CaFe]. Note that our problem is slightly different because, we are considering a spatial adiabatic problem, but some techniques may be related.

When  $\psi_0 = \hat{U} \begin{pmatrix} 0 \\ a_{-,0} \end{pmatrix}$  (resp.  $\psi_0 = \hat{U} \begin{pmatrix} a_{+,0} \\ 0 \end{pmatrix}$ ), the question is whether the solution  $\psi(t)$  to

$$i\partial_t \psi = H_{Lin} \psi + G_{\varepsilon,\tau} |\psi|^2 \psi, \quad \psi(t=0) = \psi_0$$

remains close to  $\hat{U} \begin{pmatrix} 0 \\ a_{-}(t) \end{pmatrix}$  (resp.  $\begin{pmatrix} a_{+}(t) \\ 0 \end{pmatrix}$ ) with

$$\begin{aligned} i\partial_t a_{-} &= \varepsilon^{2+2\delta} \tau_x \hat{H}_{-} a_{-} + \frac{G\varepsilon^{2+2\delta} \tau_x}{2} |a_{-}|^2 a_{-}, \quad a_{-}(t=0) = a_{-,0}, \\ \text{resp. } i\partial_t a_{+} &= \varepsilon^{2+2\delta} \tau_x \hat{H}_{+} a_{+} + \frac{G\varepsilon^{2+2\delta} \tau_x}{2} |a_{+}|^2 a_{+}, \quad a_{+}(t=0) = a_{+,0}. \end{aligned}$$

More precisely, the question is about the range of time where this approximation is valid: what is the size of  $T_\varepsilon$  w.r.t  $\varepsilon$  such that  $\sup_{t \in [-T_\varepsilon, T_\varepsilon]} \|\psi(t) - \hat{U} \begin{pmatrix} 0 \\ a_{-}(t) \end{pmatrix}\|$  (resp.  $\sup_{t \in [-T_\varepsilon, T_\varepsilon]} \|\psi(t) - \begin{pmatrix} a_{+}(t) \\ 0 \end{pmatrix}\|$ ) remains small.

Since the approximation of  $\hat{U}^* H_{Lin} \hat{U}$  by  $\begin{pmatrix} \hat{H}_{+} & 0 \\ 0 & \hat{H}_{-} \end{pmatrix}$  is good in the low frequency range, a natural assumption will be that the initial data are supported in the low frequency region

$$a_{0,\pm} = \chi(\tau_x |\varepsilon D_q|^2) a_{0,\pm},$$

for some compactly supported  $\chi$ . Then the question is whether the norm of  $(1 - \tilde{\chi}(\varepsilon^2 \tau_x D_q^2))\psi(t)$  remains small for  $t \in [0, T_\varepsilon]$  for  $\tilde{\chi} \in \mathcal{C}_0^\infty(\mathbb{R})$ ,  $\chi \prec \tilde{\chi}$ . Then the two last parts of Section 3, concerned with the high frequency part and the effect of  $\hat{U}$  on the nonlinear term, have to be reconsidered.

Note that the adiabatically prepared state with  $\psi_0 = \hat{U} \begin{pmatrix} a_{0,+} \\ 0 \end{pmatrix}$  are probably not stable for very long time,  $T_\varepsilon = \mathcal{O}(e^{\frac{\varepsilon}{\varepsilon}})$ , because the characteristic set

$$\mathcal{C}_\lambda = \{(q, p) \in \mathbb{R}^4, \quad \det(\varepsilon^{2\delta} \tau_x p^2 + V_{\varepsilon, \tau}(q) + M(q) - \lambda) = 0\}$$

contains two components when  $\lambda \geq \min E_+$ , one corresponding to the higher level of  $M(q)$  with  $|p|^2 \leq C(\lambda)$ , and another one for the lower level of  $M(q)$  but with large  $p$ 's. This means that a tunnel effect will occur between the two levels, so that adiabatically prepared states, with energies close to  $\lambda \geq \min E_+$ , will not remain in this state for (very) large times.

## A Semiclassical calculus

### A.1 Short review in the scalar case

Consider a Hörmander metric,  $g$ , that is a metric on  $\mathbb{R}_{q,p}^{2d}$ , which satisfies the uncertainty principle, the slowness and temperance conditions (see [Hor, BoLe]) and consider  $g$ -weights (slow and tempered for  $g$ )  $M, M_1, M_2$ . The symplectic form on  $\mathbb{R}_{q,p}^{2d}$  is denoted by  $\sigma$  :

$$\sigma(X, X') = \sum_{j=1}^d p^j q'_j - q_j p'^j, \quad X = (q, p), X' = (q', p').$$

The dual metric  $g^\sigma$  is given by  $g_X^\sigma(T) = \sup_{T' \neq 0} \frac{|\sigma(T, T')|^2}{g_X(T')}$  and the gain associated with  $g$  is

$$\lambda(X) = \inf_{T \neq 0} \left( \frac{g_X^\sigma(T)}{g_X(T)} \right)^{1/2} \geq 1 \quad (\text{uncertainty}). \quad (\text{A.1})$$

In the scalar case, the space  $S(M, g)$  is then the subspace of  $\mathcal{C}^\infty(\mathbb{R}_{p,q}^{2d}; \mathbb{C})$  of functions such that

$$\forall N \in \mathbb{N}, \exists C_N \sup_{g_X(T_\ell)=1} |(T_1 \dots T_N a)(X)| \leq C_N M(X),$$

after identifying a vector field  $T_\ell$  with a first-order differentiation operator. For a given  $N \in \mathbb{N}$ , the system of seminorms  $(p_{N,M,g})_{N \in \mathbb{N}}$  defined by

$$p_{N,M,g}(a) = \sup_{X \in \mathbb{R}^{2d}} \sup_{g_X(T_\ell)=1} M(X)^{-1} |(T_1, \dots, T_N a)(X)|$$

makes  $S(M, g)$  a Fréchet space.

For  $a \in \mathcal{S}'(\mathbb{R}_{q,p}^{2d})$  and  $\varepsilon > 0$ , the Weyl quantized operator  $a^W(q, \varepsilon D_q) : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}'(\mathbb{R}^d)$  is given by its kernel

$$a^W(q, \varepsilon D_q)(q, q') = \int_{\mathbb{R}^d} e^{i \frac{(q-q') \cdot p}{\varepsilon}} a\left(\frac{q+q'}{2}, p\right) \frac{dp}{(2\pi\varepsilon)^d}.$$

When no confusion is possible, we shall use the shortest notations

$$a^W(q, \varepsilon D_q) = a^W = a(q, \varepsilon D_q).$$

When  $a \in S(M, g)$ , it sends  $\mathcal{S}(\mathbb{R}^d)$  (resp.  $\mathcal{S}'(\mathbb{R}^d)$ ) into itself and the composition  $a_1 \circ a_2$  makes sense for  $a_j \in S(M_j, g)$ . The Moyal product  $a_1 \#^\varepsilon a_2$  is then defined as the Weyl-symbol of  $a_1^W(q, \varepsilon D_q) \circ a_2^W(q, \varepsilon D_q)$ :

$$\begin{aligned} a_1 \#^\varepsilon a_2(X) &= \left( e^{\frac{i\varepsilon}{2} \sigma(D_{X_1}, D_{X_2})} a_1(X_1) a_2(X_2) \right) \Big|_{X_1=X_2=X} \\ &= \sum_{j=0}^{J-1} \frac{\left( \frac{i\varepsilon}{2} \sigma(D_{X_1}, D_{X_2}) \right)^j}{j!} a_1(X_1) a_2(X_2) \Big|_{X_1=X_2=X} \\ &\quad + \int_0^1 \frac{(1-\theta)^{J-1}}{(J-1)!} e^{\frac{i\varepsilon}{2} \theta \sigma(D_{X_1}, D_{X_2})} \left( \frac{i\varepsilon}{2} \sigma(D_{X_1}, D_{X_2}) \right)^J a_1(X_1) a_2(X_2) \Big|_{X_1=X_2=X} \\ &= \sum_{j=0}^{J-1} \frac{\left( \frac{i\varepsilon}{2} \sigma(D_{X_1}, D_{X_2}) \right)^j}{j!} a_1(X_1) a_2(X_2) \Big|_{X_1=X_2=X} + \varepsilon^J R_J(a_1, a_2, \varepsilon)(X), \quad (\text{A.2}) \end{aligned}$$

where  $R_J(., ., \varepsilon)$  is a uniformly continuous bilinear operator from  $S(M_1, g) \times S(M_2, g)$  into  $S(M_1 M_2 \lambda^{-J}, g)$  (i.e. any seminorm of  $R_J(a_1, a_2, \varepsilon)$  is uniformly controlled by some bilinear expression of a finite number of seminorms of  $a_1$  and  $a_2$ ).

The three first terms of the previous expansion are given by

$$\begin{aligned} a_1 \#^\varepsilon a_2 &= a_1 a_2 + \frac{\varepsilon}{2i} [\partial_{p_k} a_1 \partial_{q^k} a_2 - \partial_{q^k} a_1 \partial_{p_k} a_2] \\ &\quad - \frac{\varepsilon^2}{8} \left[ (\partial_{p_k, p_\ell}^2 a_1) (\partial_{q^k, q^\ell}^2 a_2) + (\partial_{q^k, q^\ell}^2 a_1) (\partial_{p_k, p_\ell}^2 a_2) - 2(\partial_{p_k, q^\ell}^2 a_1) (\partial_{q^k, p_\ell}^2 a_2) \right] \quad (\text{A.3}) \\ &\quad + \varepsilon^3 R_3(a_1, a_2, \varepsilon), \end{aligned}$$

by making use of the Einstein convention  $s^j t_j = \sum_j s^j t_j$ .

**Definition A.1.** *With the small parameter  $\varepsilon \in (0, \varepsilon_0)$ , it is more convenient to consider the Fréchet-space  $S_u(M, g)$  of bounded functions from  $(0, \varepsilon_0)$  to  $S(M, g)$  endowed with the seminorms:*

$$P_{N, M, g}(a) = \sup_{\varepsilon \in (0, \varepsilon_0)} p_{N, M, g}(a(\varepsilon)).$$

*The subscript  $_u$  stands for uniform seminorm estimates.*

*The space of  $\varepsilon$ -quantized family of symbols will be denoted by  $OpS_u(M, g)$ :*

$$(a(\varepsilon) \in S_u(M, g)) \Leftrightarrow (a^W(q, \varepsilon D_q, \varepsilon) \in OpS_u(M, g)).$$

We shall give a variation of this definition in Subsection A.4 below for parameter dependent metrics.

We recall the Beals-criterion proved in [BoCh] (see [NaNi] for the  $\varepsilon$ -dependent version) for diagonal Hörmander metrics of the form  $g = \sum_{j=1}^d \frac{dq_j'^2}{\varphi_j(X)^2} + \frac{dp_j^2}{\psi_j(X)^2}$ . Set  $\mathfrak{D} = (D_{q^1}, \dots, D_{q^d}, q^1, \dots, q^d)$  and for  $E \in \mathbb{N}^{2d}$  introduce the multi-commutator  $\text{ad}_{\mathfrak{D}}^E = \prod_{j=1}^{|E|} \text{ad}_{\mathfrak{D}_j}^{E_j}$  acting on the continuous operators from  $\mathcal{S}(\mathbb{R}^d)$  to  $\mathcal{S}'(\mathbb{R}^d)$  and the weight  $M_E(X) = (\varphi(X), \psi(X))^E$ . Then the Beals criterion says that an operator  $A : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}'(\mathbb{R}^d)$  belongs to  $OpS(1, g)$  if and only if

$$\text{ad}_{\mathfrak{D}}^E A \in \mathcal{L}(L^2(\mathbb{R}^d), H^\varepsilon(M_E))$$

for all  $E \in \mathbb{N}^{2d}$ , when the Sobolev space  $H^\varepsilon(M_E)$  is given by

$$\|u\|_{H^\varepsilon(M_E)} = \|M_E(q, \varepsilon D_q)u\|_{L^2}.$$

Moreover the family of seminorms  $(Q_N)_{N \in \mathbb{N}}$ , defined by,

$$Q_N(A) = \sup_{\varepsilon \in (0, \varepsilon_0)} \max_{|E|=N} \varepsilon^{-N} \|\text{ad}_{\mathfrak{D}}^E A(\varepsilon)\|_{\mathcal{L}(L^2(\mathbb{R}^d), H^\varepsilon(M_E, g))} \quad (\text{A.4})$$

on  $OpS_u(M, g)$ , is uniformly equivalent to the family  $(P_N(a))_{N \in \mathbb{N}}$  on  $S_u(M, g)$  after the identification  $A(\varepsilon) = a^W(q, \varepsilon D_q, \varepsilon)$ . “Uniformly” means here that the comparison of the two topologies is expressed with constants independent of  $\varepsilon \in (0, \varepsilon_0)$ .

Below is an example of a metric which satisfies all the assumptions and which is used in our computations

$$g = \frac{dq'^2}{(1 + |q'|^2)^\varrho} + dq''^2 + \frac{dp^2}{(1 + |p|^2)^{\varrho'}}, \quad m \geq 0, \quad \varrho, \varrho' \in [0, 1], \quad (\text{A.5})$$

with the gain function  $\lambda(q, p) = \langle p \rangle^{\varrho'}$ .

It is convenient to introduce the class of negligible symbols and operators.

**Definition A.2.** An element  $a \in S_u(1, g)$ , belongs to  $\mathcal{N}_{u, g}$  if

$$\forall N, N' \in \mathbb{N}, \exists C_{N, N'} > 0, \quad \varepsilon^{-N} a(\varepsilon) \in S_u(\lambda^{-N'}, g).$$

Similarly,  $Op\mathcal{N}_{u, g}$  denotes the  $\varepsilon$ -quantized version:

$$(a^W(q, \varepsilon D_q, \varepsilon) \in Op\mathcal{N}_{u, g}) \Leftrightarrow (a \in \mathcal{N}_{u, g}).$$

Combined with the following relation between cut-off functions it provides easy estimates from phase-space localization.

**Definition A.3.** For two cut-off functions  $\chi_1, \chi_2 \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$ ,  $0 \leq \chi_{1,2} \leq 1$ , the notation  $\chi_1 \prec \chi_2$  means that  $\chi_2 \equiv 1$  in a neighborhood of  $\text{supp } \chi_1$ .

For example the pseudodifferential calculus leads to

$$(\chi_1 \prec \chi_2) \Rightarrow (\forall a \in S_u(M, g), \quad (1 - \chi_2)^\# a^\# \chi_1 \in \mathcal{N}_{u, g}), \quad (\text{A.6})$$

when the weight  $M$  satisfies  $M \leq C\lambda^C$  for some  $C > 0$ .

## A.2 Applications to matricial operators

Operator valued pseudodifferential calculus has been studied in [Bak]. When  $\mathfrak{h}$  is a Hilbert space it suffices to tensorize the previous calculus with  $\mathcal{L}(\mathfrak{h})$ , which corresponds to the componentwise definition in  $\mathcal{M}_n(\mathbb{C})$  when  $\mathfrak{h} = \mathbb{C}^n$ . The corresponding class of symbols associated with a Hörmander metric  $g$  and a  $g$ -tempered weight  $M$  is denoted by  $S(M, g; \mathcal{L}(\mathfrak{h}))$  while the set of bounded families in  $S(M, g; \mathcal{L}(\mathfrak{h}))$  parametrized by  $\varepsilon \in (0, \varepsilon_0)$  is denoted by  $S_u(M, g; \mathcal{L}(\mathfrak{h}))$ . The asymptotic expansions (A.2)-(A.3) of the Moyal product clearly holds (see [PST] for a presentation without specifying the remainder terms) if one takes care of the order of the symbols. For example, the two first terms of the expansion of a commutator  $[a_1(q, \varepsilon D_q), a_2(q, \varepsilon D_q)]$  are

$$\begin{aligned} a_1 \#^\varepsilon a_2 - a_2 \#^\varepsilon a_1 &= [a_1(q, p), a_2(q, p)] \\ &+ \frac{\varepsilon}{2i} (\partial_p a_1 \partial_q a_2 - \partial_q a_1 \partial_p a_2) - \frac{\varepsilon}{2i} (\partial_p a_2 \partial_q a_1 - \partial_q a_2 \partial_p a_1) \\ &+ \varepsilon^2 [R_2(a_1, a_2, \varepsilon) - R_2(a_2, a_1, \varepsilon)] \quad (\text{A.7}) \end{aligned}$$

with no simpler expression when the matricial symbols do not commute.

When the Hörmander metric  $g$  has the form  $\sum_j \frac{dq_j^2}{\varphi_j^2} + \frac{dp_j^2}{\psi_j^2}$  the uniform Beals criterion also holds: In the seminorms  $Q(a)$  defined in (A.4) simply replace  $L^2(\mathbb{R}^d)$  by the Hilbert tensor product  $L^2(\mathbb{R}^d) \otimes \mathfrak{h}$  and consider the operators  $\mathfrak{D}$  and  $M_E(q, \varepsilon D_q)$  as the diagonal ones  $\mathfrak{D} \otimes \text{Id}_{\mathfrak{h}}$  and  $M_E(\cdot, \varepsilon D_q) \otimes \text{Id}_{\mathfrak{h}}$ . Finally the Definition A.2 of negligible symbols also makes sense for matricial symbols after replacing  $OpS(\lambda^{-N'}, g)$  by  $OpS(\lambda^{-N'}, g; \mathcal{L}(\mathfrak{h}))$ .

We end this section with standard applications of the Beals criterion.

**Proposition A.4.** *Consider a diagonal Hörmander metric  $g = \sum_{j=1}^d \frac{dq_j^2}{\varphi_j(X)^2} + \frac{dp_j^2}{\psi_j(X)^2}$  and the constant metric  $g_0 = dq^2 + dp^2$ . Assume that any  $f$  chosen in  $\{\varphi_j, \psi_j, j \in \{1, \dots, d\}\}$  is a  $g_0$ -slow and -tempered weight such that  $f(q, \varepsilon D_q)^s$  belongs  $OpS_u(f^s, g_0)$  for any  $s \in \mathbb{N}$ .<sup>2</sup>*

*Assume that  $A \in OpS_u(1, g; \mathcal{L}(\mathfrak{h}))$  is a family of invertible operators in  $\mathcal{L}(L^2(\mathbb{R}^d) \otimes \mathfrak{h})$  and such that  $\|A^{-1}(\varepsilon)\|$  is uniformly bounded in w.r.t  $\varepsilon \in (0, \varepsilon_0)$ . Then  $A^{-1}$  belongs to  $OpS_u(1, g; \mathcal{L}(\mathfrak{h}))$ .*

**Proof:** We start from the relation

$$\text{ad}_{\mathfrak{D}}^E A^{-1} = \sum_{|E'|=|E|, E' \in \mathbb{N}^{|E|}} c_{E, E'} A^{-1} \prod_{j=1}^{|E|} \left[ \left( \text{ad}_{\mathfrak{D}}^{E'_j} A \right) A^{-1} \right]. \quad (\text{A.8})$$

which holds in  $\mathcal{L}(L^2(\mathbb{R}^d) \otimes \mathfrak{h})$  for all  $E \in \mathbb{N}^{2d}$ . Hence the Beals criterion in the metric  $g_0$  says that  $A^{-1}$  belongs to  $OpS_u(1, g; \mathcal{L}(\mathfrak{h}))$ . In particular  $A^{-1}$  belongs to  $\mathcal{L}(H^\varepsilon(M_{E''}))$  for any  $E'' \in \mathbb{N}^{2d}$ . This allows to apply the Beals criterion in the metric  $g$  and yields the result.  $\square$

<sup>2</sup>This last condition is redundant after a possible modification of  $\varphi_j$  and  $\psi_j$  if one refers to [BoCh], but easier to check directly in our examples than giving the general proof.

### A.3 Pseudodifferential projections

An application of the Beals criterion says that a true pseudodifferential projection can be made from an approximate one at the principal symbol level. This holds for matricial symbols.

**Proposition A.5.** *Consider a diagonal Hörmander metric  $g = \sum_{j=1}^d \frac{dq_j^2}{\varphi_j(X)^2} + \frac{dp_j^2}{\psi_j(X)^2}$  with the same properties as in Proposition A.4. Assume that the operator  $\hat{\Pi} \in OpS_u(1, g; \mathcal{L}(\mathfrak{h}))$  satisfies*

$$\left( \hat{\Pi} \circ \hat{\Pi} - \hat{\Pi} \right) = \varepsilon^\mu \hat{R}_\mu + \varepsilon^\nu \hat{R}_\nu,$$

with  $R_\mu \in S_u(M, g; \mathcal{L}(\mathfrak{h}))$ ,  $R_\nu \in S_u(N, g; \mathcal{L}(\mathfrak{h}))$ ,  $\nu > \mu > 0$  and  $M, N \leq 1$ . Assume additionally that there exist  $\chi, \chi' \in S_u(1, g; \mathcal{L}(\mathfrak{h}))$ ,  $0 \leq \chi \leq \chi' \leq 1$  such that  $\chi \prec \chi'$  and  $\chi' R_\mu = 0$ .

Then for  $\varepsilon_1 \leq \varepsilon_0$  small enough, the operator

$$\hat{P} = \frac{1}{2i\pi} \int_{|z-1|=1/2} (z - \hat{\Pi})^{-1} dz$$

is well defined for  $\varepsilon \in (0, \varepsilon_1)$  and satisfies

$$\begin{aligned} \hat{P} \circ \hat{P} &= \hat{P} \quad \text{in} \quad \mathcal{L}(L^2(\mathbb{R}^d) \otimes \mathfrak{h}), \\ \text{and} \quad (\hat{P} - \hat{\Pi}) &= \varepsilon^\mu \hat{\Pi}_\mu + \varepsilon^\nu \hat{\Pi}_\nu. \end{aligned}$$

with  $\Pi_\mu \in S_u(M, g; \mathcal{L}(\mathfrak{h}))$ ,  $\Pi_\nu \in S_u(N, g; \mathcal{L}(\mathfrak{h}))$  and  $\hat{\Pi}_\mu \circ \hat{\chi} \in Op\mathcal{N}_{u,g}$ .

**Proof:** The first result concerned with the definition of  $\hat{P}$  is a direct application of the simple general result in Lemma A.6 applied with  $T = \hat{\Pi}$  and  $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathfrak{h}$ . Note that our assumptions  $\nu > 1$  and  $M \leq 1$  ensure that  $\|\hat{\Pi}^2 - \hat{\Pi}\| \leq \frac{1}{8}$  as soon as  $\varepsilon \leq \varepsilon_1$  with  $\varepsilon_1$  small enough.

Writing

$$\hat{\Pi} - \hat{P} = (\hat{\Pi}^2 - \hat{\Pi})(A_1 - A_0)$$

with

$$A_x = \frac{1}{2i\pi} \int_{|z-x|} (z - \hat{\Pi})^{-1} dz, \quad x \in \{0, 1\},$$

reduces the problem to proving

$$A_x \in OpS_u(1, g; \mathcal{L}(\mathfrak{h})) \quad \text{or} \quad (z - \hat{\Pi})^{-1} \in OpS_u(1, g; \mathcal{L}(\mathfrak{h})),$$

when  $\{|z-x|=1/2\}$  with uniform bounds. But this was proved in Proposition A.4 as a consequence of the Beals criterion. This ends the proof.  $\square$

**Lemma A.6.** Assume that in an Hilbert space  $\mathcal{H}$ , the operator  $T \in \mathcal{L}(\mathcal{H})$  satisfies  $\|T^2 - T\| \leq \delta < 1/4$  and  $\|T\| \leq C$ . Then there exists  $c_\delta < \frac{1}{2}$  such that

$$\sigma(T) \subset \{z \in \mathbb{C}, |z(z-1)| \leq \delta\} \subset \{z \in \mathbb{C}, |z| \leq c_\delta\} \cup \{z \in \mathbb{C}, |z-1| \leq c_\delta\},$$

$$\max \left\{ \|(z-T)^{-1}\|, |z-1| = \frac{1}{2} \right\} \leq 2 \frac{2C+1}{1-4\delta}.$$

Moreover, the operator

$$P = \frac{1}{2i\pi} \int_{|z-1|=1/2} (z-T)^{-1} dz.$$

differs from  $T$  according to

$$T - P = (T^2 - T)(A_1 - A_0) = (A_1 - A_0)(T^2 - T), \quad (\text{A.9})$$

$$\text{with } A_1 = \frac{1}{2i\pi} \int_{|z-1|=1/2} (T-z)^{-1}(1-z)^{-1} dz \quad (\text{A.10})$$

$$\text{and } A_0 = \frac{1}{2i\pi} \int_{|z|=1/2} (T-z)^{-1} z^{-1} dz. \quad (\text{A.11})$$

**Proof:** If  $z \in \sigma(T)$  then  $z(z-1) \in \sigma(T(T-1)) \subset \{z \in \mathbb{C}, |z(z-1)| \leq \frac{1}{4}\}$  (Remember that  $|z(z-1)| = \frac{1}{4}$  means  $|Z - \frac{1}{4}| = \frac{1}{4}$  with  $Z = (z - \frac{1}{2})^2$ ). Consider  $z \in \mathbb{C}$  such that  $|z-1| = \frac{1}{2}$ , then the relation

$$(T-z)(T-(1-z)) = z(1-z) + (T^2 - T),$$

with  $|z(1-z)| \geq \frac{1}{4}$  and  $\|T^2 - T\| \leq \delta < \frac{1}{4}$ , implies

$$\|(T-z)^{-1}\| \leq \|T-(1-z)\| \|[z(1-z) + T^2 - T]^{-1}\| \leq \frac{C + \frac{1}{2}}{\frac{1}{4} - \delta} \quad \text{for } |z-1| = \frac{1}{2}.$$

The symmetry with respect to  $z = \frac{1}{2}$  due to  $(1-T)(1-T) - (1-T) = T^2 - T$  implies also

$$\|(T-z)^{-1}\| \leq \frac{C + \frac{1}{2}}{\frac{1}{4} - \delta} \quad \text{for } |z| = \frac{1}{2}.$$

Compute

$$\begin{aligned} T - P &= \frac{1}{2i\pi} \int_{|z-1|=1/2} [T(z-1)^{-1} - (z-T)^{-1}] dz \\ &= (T-1)P + (T^2 - T)A_1 \\ \text{with } A_1 &= \frac{1}{2i\pi} \int_{|z-1|=1/2} (T-z)^{-1}(1-z)^{-1} dz. \end{aligned}$$

In particular this implies to  $T(1-P) = (T^2 - T)A_1$  while replacing  $T$  with  $(1-T)$  and  $P$  with  $1-P$  leads to

$$P - T = -T(1-P) + (T^2 - T)A_0 \quad \text{with } A_0 = \frac{1}{2i\pi} \int_{|z|=1/2} (T-z)^{-1} z^{-1} dz.$$



Summing the two previous identities yields the result.  $\square$

#### A.4 Extension to parameter dependent metrics

Additionally to the semiclassical (or adiabatic) parameter, we need other parameters  $\tau = (\tau', \tau'') \in (0, 1]^2$  on which the metric  $g = g_\tau$  depends. In general consider  $\tau \in \mathcal{T} \subset \mathbb{R}^\nu$  and a family of Hörmander metrics  $(g_\tau)_{\tau \in \mathcal{T}}$  defined on  $\mathbb{R}_{q,p}^{2d}$ .

**Definition A.7.** *The family of metrics  $(g_\tau)_{\tau \in \mathcal{T}}$  is said admissible if the uncertainty principle (A.1) is satisfied and if the slowness and temperance constants  $C_1, C_2, N_2$  involved in*

$$\begin{aligned} (\text{slowness}) \quad & \left( g_{\tau,X}(X - Y) \leq \frac{1}{C_1} \right) \Rightarrow \left( \left( \frac{g_{\tau,X}}{g_{\tau,Y}} \right)^{\pm 1} \leq C_1 \right), \\ (\text{temperance}) \quad & \left( \frac{g_{\tau,X}}{g_Y} \right)^{\pm 1} \leq C_2(1 + g_{\tau,X}^\sigma(X - Y))^{N_2}, \end{aligned}$$

can be chosen uniformly w.r.t  $\tau \in \mathcal{T}$ .

Accordingly a family of weights  $(M_\tau)_{\tau \in \mathcal{T}}$  will be admissible if the slowness and temperance constants of  $M_\tau$  w.r.t  $g_\tau$  can be chosen uniform w.r.t  $\tau \in \mathcal{T}$ .

The important point is that all the estimates of the Weyl-Hörmander pseudodifferential calculus (see [Hor, BoLe]), including the equivalence of norms in the Beals criterion of [BoCh], occur with constants which are determined by the dimension  $d$ , the uncertainty lower bound (which is 1 here), the slowness and temperance constants. Hence all the pseudodifferential and semiclassical estimates, (operator norms or seminorms of remainder terms) are uniform w.r.t to  $(\varepsilon, \tau)$  as long as the symbols,  $a_k(\varepsilon, \tau)$ ,  $k = 1, 2$ , have uniformly controlled seminorm in  $S(M_{\tau,k}, g_\tau)$ , w.r.t  $(\varepsilon, \tau) \in (0, \varepsilon_0] \times \mathcal{T}$ .

The definition of symbol classes  $S_u(M, g)$  with uniform control of seminorms w.r.t  $\varepsilon \in (0, \varepsilon_0]$  can be extended to admissible families  $(M_\tau, g_\tau)_{\tau \in \mathcal{T}}$ .

**Definition A.8.** *For an admissible family  $(M_\tau, g_\tau)_{\tau \in \mathcal{T}}$ , the set of parameter dependent symbol  $a(X, \varepsilon, \tau)$ ,  $X \in \mathbb{R}^{2d}$ ,  $(\varepsilon, \tau) \in (0, \varepsilon_0] \times \mathcal{T}$  with uniform estimates*

$$\forall N \in \mathbb{N}, \exists C_N > 0, \forall (\varepsilon, \tau) \in (0, \varepsilon_0] \times \mathcal{T}, \quad p_{N, M_\tau, g_\tau}(a(\varepsilon, \tau)) \leq C_N,$$

is denoted by  $S_u(M_\tau, g_\tau, \mathcal{L}(\mathbf{h}))$ ,  $\tau \in \mathcal{T}$ .

Equivalently the set of semiclassically quantized operators  $a(q, \varepsilon D_q, \varepsilon, \tau)$  when the symbol  $a$  belongs to  $S_u(M_\tau, g_\tau; \mathcal{L}(\mathbf{h}))$  is denoted by  $OpS_u(M_\tau, g_\tau; \mathcal{L}(\mathbf{h}))$ .

The set of negligible symbols and operators associated with  $(g_\tau)_{\tau \in \mathcal{T}}$  with uniform estimates in Definition A.2 w.r.t  $\tau \in \mathcal{T}$  is denoted by  $\mathcal{N}_{u, g_\tau}$  and  $Op\mathcal{N}_{u, g_\tau}$ .

**Proposition A.9.** *For  $\tau = (\tau', \tau'') \in (0, 1]^2$  the family  $(g_\tau)_{\tau \in (0, 1]^2}$  defined on  $\mathbb{R}^{2d} = \mathbb{R}^{2(d'+d'')}$  by*

$$g_\tau = \frac{\tau' dq'^2}{\langle \sqrt{\tau'} q' \rangle^2} + \tau'' dq''^2 + \frac{\tau' \tau'' dp^2}{\langle \sqrt{\tau' \tau''} p \rangle^2}$$

is admissible.

**Proof:** It is easier to consider the symplectically equivalent metric (use the transform  $(q', q'', p', p'') \rightarrow (\tau'^{\frac{1}{2}} q', \tau''^{\frac{1}{2}} q'', \tau'^{-\frac{1}{2}} p', \tau''^{-\frac{1}{2}} p'')$ )

$$\tilde{g}_\tau = \frac{dq'^2}{\langle q' \rangle^2} + dq'' + \frac{\tau'^2 dp'^2 + \tau''^2 dp''^2}{\langle p \rangle_\tau^2}$$

after setting  $\langle p \rangle_\tau^2 = 1 + \tau'^2 p'^2 + \tau''^2 p''^2$ . Firstly remember that the metric

$$g_{(1,1)} = \frac{dq'^2}{\langle q' \rangle^2} + dq'' + \frac{dp^2}{\langle p \rangle^2}.$$

is a Hörmander metric. The metric  $\tilde{g}_\tau^\sigma$  is given by

$$\tilde{g}_\tau^\sigma = \frac{\langle p \rangle_\tau^2}{\tau'^2} dq'^2 + \frac{\langle p \rangle_\tau^2}{\tau''^2} dq''^2 + \langle q' \rangle^2 dp'^2 + dp''^2.$$

Hence the uncertainty principle (A.1) is satisfied with

$$\lambda_\tau(q', q'', p', p'') = \min \left\{ \langle q' \rangle \frac{\langle p \rangle_\tau}{\tau'}, \frac{\langle p \rangle_\tau}{\tau''} \right\} \geq \langle p \rangle_\tau \geq 1.$$

In order to check the uniform slowness and temperance of  $\tilde{g}_\tau$ , introduce the new variables  $X_\tau = (q', q'', \tau' p', \tau'' p'')$  when  $X = (q', q'', p', p'')$  with a similar definition for  $Y_\tau$  and  $T_\tau$ .

**Slowness:** Write

$$\left( \tilde{g}_{\tau,X}(X - Y) \leq \frac{1}{C_1} \right) \Leftrightarrow \left( \tilde{g}_{(1,1),X_\tau}(X_\tau - Y_\tau) \leq \frac{1}{C_1} \right).$$

When  $C_1$  is slowness constant of  $\tilde{g}_{(1,1)}$ , this implies

$$\left( \frac{\tilde{g}_{(1,1),X_\tau}}{\tilde{g}_{(1,1),Y_\tau}} \right)^{\pm 1} \leq C_1$$

which is nothing but

$$\left( \frac{\tilde{g}_{\tau,X}}{\tilde{g}_{\tau,Y}} \right)^{\pm 1} \leq C_1.$$

**Temperance:** Write

$$\left( \frac{\tilde{g}_{\tau,X}(T)}{\tilde{g}_{\tau,Y}(T)} \right)^{\pm 1} = \left( \frac{\tilde{g}_{(1,1),X_\tau}(T_\tau)}{\tilde{g}_{(1,1),Y_\tau}(T_\tau)} \right)^{\pm 1} \leq C_2 (1 + \tilde{g}_{(1,1),X_\tau}^\sigma(X_\tau - Y_\tau))^{N_2},$$

when  $C_2$  and  $N_2$  are the temperance constants for  $\tilde{g}_{(1,1)}$ . The problem is reduced to showing

$$\forall X, T \in \mathbb{R}^{2d}, \quad \tilde{g}_{(1,1),X_\tau}^\sigma(T_\tau) \leq \tilde{g}_{\tau,X}^\sigma(T).$$

The expression of  $\tilde{g}_\tau^\sigma$  gives with  $X = (q', q'', p', p'')$  and  $T = (\theta', \theta'', \pi', \pi'')$

$$\tilde{g}_{(1,1),X_\tau}^\sigma(T_\tau) = \langle p \rangle_\tau^2 \theta'^2 + \langle p \rangle_\tau^2 \theta''^2 + \langle q' \rangle^2 \tau'^2 \pi'^2 + \tau''^2 \pi''^2 \leq \tilde{g}_{\tau,X}^\sigma(T)$$

owing to  $\max\{\tau', \tau''\} \leq 1$ .

□

**Acknowledgements:** The authors are very grateful to Jean Dalibard for explaining the mathematical questions arising from a two level atom in a light beam and for many detailed discussions that took place for the duration of this work. They also wish to thank G. Panati, C. Lebris and S.V. Ngoc for their occasional help. This work was initiated while the second author had a CNRS-sabbatical semester at CMAP in Ecole Polytechnique. They acknowledge support from the French ministry Grant ANR-BLAN-0238, VoLQuan.

## References

- [Aft] A. Aftalion. *Vortices in Bose-Einstein Condensates*. Progress in Nonlinear Differential Equations and their Applications, Vol 67 Birhkaüser (2006).
- [AB] A. Aftalion, X. Blanc. Reduced energy functionals for a three dimensional fast rotating Bose Einstein condensates. *Ann. Inst. H. Poincaré Anal. Non Linéaire* 25 no. 2 (2008), pp 339-355.
- [ABN] A. Aftalion, X. Blanc, F. Nier. Lowest Landau level functional and Bargmann spaces for Bose-Einstein condensates. *J. Funct. Anal.* 241 no. 2 (2006), pp 661-702.
- [AJR] A. Aftalion, R. L. Jerrard, J. Royo-Letelier. Non existence of vortices in the small density region of a condensate *Jour. Funct. Anal.*, vol. 260, no. 8 (2011), pp 2387-2406.
- [Bak] A. Balazard-Konlein. Calcul fonctionnel pour des opérateurs  $h$ -admissible à symbole opérateur et applications. ph-D, Université de Nantes, (1985).
- [BCR] J. Bochnak, M. Coste, M.F. Roy. *Géométrie algébrique réelle*. *Ergebnisse der Mathematik und ihrer Grenzgebiete* (3), 12 Springer-Verlag (1987).
- [BDLM] J. Bolte, A. Daniilidis, O. Ley, L. Mazet. Characterizations of Łojasiewicz inequalities and applications: subgradient flows, talweg, convexity. *Math. Oper. Res.* 36 no. 1 (2011), pp 55-70.
- [BoCh] J.M. Bony, J.Y. Chemin. Espaces fonctionnels associés au calcul de Weyl-Hörmander. *Bull. Soc. Math. France*, 122 no 1 (1994), pp 77-118.
- [BoFo] M. Born, V.Fock. Beweis des Adiabatsatzes. *Zeitschrift für Physik* 51 (1928), pp 165-169.
- [BoLe] J.M. Bony, N. Lerner. Quantification asymptotique et microlocalisation d'ordre supérieur I. *Ann. Scient. Ec. Norm. Sup.*, 4<sup>e</sup> série 22 (1989), pp 377-433.
- [BoOp] M. Born, R. Oppenheimer. Zur Quantentheorie der Molekeln. *Ann. Phys. (Leipzig)* 84 (1927), pp 457-484.

- [BrOs] H. Brezis, L. Oswald. Remarks on sublinear elliptic equations, *Nonlinear Analysis* 10 (1986), pp 55–64.
- [CaFe] R. Carles, C. Fermanian. A nonlinear adiabatic theorem for coherent states. *Nonlinearity* 24 no. 8 (2011), pp 2143–2164.
- [CFKS] H.L. Cycon, R.G. Froese, W. Kirsch, B. Simon. *Schrödinger operators with application to quantum mechanics and global geometry*. Texts and Monographs in Physics. Springer Study Edition. Springer-Verlag (1987).
- [Chi] R. Chill. On the Łojasiewicz-Simon gradient inequality. *J. Funct. Anal.* 201 no. 10 (2003), pp 572–601.
- [Coo] N.R. Cooper. Rapidly Rotating Atomic Gases *Advances in Physics* 57 (2008), p 539.
- [DGJO] J. Dalibard, F. Gerbier, G. Juzeliūnas, P. Öhberg. Artificial gauge potentials for neutral atoms. *Rev. Mod. Phys.* 83 (2011), p 1523.
- [Fet] A.L. Fetter. Rotating trapped Bose-Einstein condensates *Rev. Mod. Phys.* 81 (2009), p 647.
- [LCGPS] Y.J. Lin, R.L. Compton, K.J. Garcia, J.V. Porto, I.B. Spielman. Synthetic magnetic fields for ultracold neutral atoms *Nature* 462 (2009), p 628
- [GCYRD] K.J. Günter, M. Cheneau, T. Yefsah, S.P. Rath, J. Dalibard. Practical scheme for a light-induced gauge field in an atomic Bose gas. *Phys. Rev. A* 79 (2009), p 011604(R).
- [HaJe] A. Haraux, M.A. Jendoubi. The Łojasiewicz gradient inequality in the infinite-dimensional Hilbert space framework. *J. Funct. Anal.* 260 no. 9 (2011), pp 2826–2842.
- [HiPr] M. Hitrik, K. Pravda-Starov. Spectra and semigroup smoothing for non-elliptic quadratic operators. *Mathematische Annalen*, 344 (2009), no.4, pp 801–846.
- [Hor] L. Hörmander. *The analysis of linear partial differential operators*. Springer Verlag (1985).
- [Hua] S.Z. Huang. *Gradient inequalities. With applications to asymptotic behavior and stability of gradient-like systems*. Mathematical Surveys and Monographs, 126. Am. Math. Soc. (2006).
- [Kat] T. Kato. *Perturbation theory for linear operators*. Reprint of the 1980 edition. Classics in Mathematics. Springer-Verlag, (1995).
- [LiSe] E.H. Lieb, R. Seiringer. Derivation of the Gross-Pitaevskii Equation for Rotating Bose Gases. *Commun. Math. Phys.* 264 (2006), pp 505–537.

- [Loj] S. Łojasiewicz. Une propriété topologique des sous-ensembles analytiques réels. *Les Equations aux Dérivées Partielles*, pp. 87-89, Editions du centre National de la Recherche Scientifique (1963).
- [MCWD1] K.W. Madison, F. Chevy, W. Wohlleben, J. Dalibard. Vortex formation in a stirred Bose-Einstein condensate. *Phys. Rev. Lett.* 84 (2000), p 806.
- [MCWD2] K. W. Madison, F. Chevy, W. Wohlleben, J. Dalibard. Vortices in a stirred Bose-Einstein condensate *Jour. Mod. Optics* 47 (2000), p 2715.
- [MaSo] A. Martinez, V. Sordoni. A general reduction scheme for the time-dependent Born-Oppenheimer approximation. *C.R. Acad. Sci. Paris Ser. I*, 334 (2002), pp 185–188.
- [MaSo2] A. Martinez, V. Sordoni. Twisted Pseudodifferential Calculus and Application to the Quantum Evolution of Molecules. *Mem. Amer. Math. Soc.* 200 no. 936 (2009).
- [NaNi] F. Nataf, F. Nier. Convergence of domain decomposition methods via semi-classical calculus. *Comm. Partial Differential Equations* 23 no. 5-6 (1998), pp 1007–1059.
- [NeSo] G. Nenciu, V. Sordoni. Semiclassical limit for multistate Klein-Gordon systems: almost invariant subspaces, and scattering theory. *J. Math. Phys.* 45 no. 9 (2004), pp 3676–3696.
- [Nie] F. Nier. A propos des fonctions  $\theta$  et des réseaux d'Abrikosov. *Séminaire Equations aux Dérivées Partielles. Ecole Polytechnique*, 2006–2007, Exp. No. XII.
- [PST] G. Panati, H. Spohn, S. Teufel. Space adiabatic perturbation theory. *Adv. Theor. Math. Phys.* 7 no. 1 (2003), pp 145–204.
- [PST2] G. Panati, H. Spohn, S. Teufel. The time-dependent Born-Oppenheimer approximation. *M2AN* 45 no. 2 (2007), pp 297–314.
- [Sim] L. Simon. Asymptotics for a class of non-linear evolution equations, with applications to geometric problems. *Ann. of Math.* 118 (1983), pp 525–571.
- [Sjo] J. Sjöstrand. Parametrix for pseudodifferential operators with multiple characteristics. *Ark. für Mat.* 12 (1974) pp 85–130.
- [Sor] V. Sordoni. Reduction scheme for semiclassical operator-valued Schrödinger type equation and application to scattering. *Comm. Partial Differential Equations* 28 no. 7-8 (2003), pp 1221–1236.
- [Tay] M. Taylor. *Partial Differential Equations III, Nonlinear Equations*. Applied Mathematical Sciences Vol. 117, Springer (1997).